

**PEER REVIEW OF THE
SAPRC-07 CHEMICAL MECHANISM OF
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Chapter 1. Summary of Conclusions

The SAPRC-07 mechanism and its documentation were taken from Dr. Carter's website (<http://www.engr.ucr.edu/~carter/SAPRC/>). The specific version of the mechanism reviewed was "SAPRC07B Mechanism; Created from Mech07.XLS 4-Jul-2008". The documentation used was William P. L. Carter "Development of a Condensed SAPRC-07 Chemical Mechanism," Report to the California Air Resources Board, Contract No. 05-750, July 4, 2008.

Chemical Species

The number and type of chemical species in SAPRC07 appear to be consistent with the state-of-the-science. The version of SAPRC07 used in this review includes 136 model species. The greater the number of species in the mechanism the greater the computational resources in terms of time and storage are required. The size of the mechanism not only affects the chemical kinetics calculations but it affects the computational resources required to calculate advection and other routines (such as deposition and aerosols). A well-balanced model will devote appropriate computational resources to each process modeled. A reasonable size for a chemical mechanism increases as computers become faster and memory becomes cheaper. At this time the number of species in SAPRC-07 is consistent with the requirements of urban and regional photochemical models. The version of the SAPRC-07 reviewed can provide the adequate level of detail that is consistent with currently available computational resources. It should be stated that Dr. Carter has more detailed sub-mechanisms that have been used for the assessment of reactivity. This is an important positive aspect of the SAPRC family of mechanisms. The SAPRC mechanism reviewed here can be easily adapted to include more species if desired for a particular application.

The species and chemical reactions included in a chemical mechanism are its building blocks. SAPRC-07 and RADM2 share a more explicit, aggregated molecule approach. CB05 was originally based on species that reflected the concentrations of organic functional groups in a given air sample but it has evolved become closer to the aggregated molecular approach used in SAPRC-07 and RACM2. To evaluate the SAPRC-07 chemical species and to better compare them with those in CB05 and RACM2 the species of all three mechanisms were lined-up side by side. This comparison is shown in the table at the end of Chapter 2. The reactions of SAPRC-07, CB05 and RACM2 were also lined-up side by side and this comparison of the reactions is shown in the table in Appendix A.

Inorganic Reactions

SAPRC-07 is well within the state of the science. All three mechanisms incorporate these basic inorganic reactions but there are some differences. At

300 K the rate constant of SAPRC-07 is greater than RACM2 by 14%. SAPRC-07 includes several reactions of ground state oxygen atom (O^3P) that may not be necessary.

Alkene Reactions

Overall the treatment of alkenes is within the state-of-the-science in SAPRC-07.

For the reaction of ozone with alkenes there remains some uncertainty in the decomposition products of the Criegee intermediate. More laboratory research in this area would be helpful.

SAPRC-07 includes the reaction of ground state oxygen atom with alkenes but RACM2 does not. This may be a remnant of environmental chamber testing; it probably is not significant under most atmospheric conditions.

Terpene Reactions

SAPRC-07 includes only one terpene species. RACM2 has a more detailed reaction scheme; RACM2 includes one species for α -pinenes and other cyclic terpenes with one double bond and a second species for d-limonene and other cyclic diene-terpenes. This should be improved in future versions of SAPRC.

Acetylene Reactions

SAPRC-07 also includes the reaction of ozone with acetylene. This is a worthwhile addition to the mechanism given that it adds no extra species to the mechanism.

Aromatic Reactions

Aromatic chemistry remains very difficult to characterize due to its complexity and its many remaining scientific uncertainties. The divergence between the three mechanisms is great. The RACM2 approach is somewhat easier to understand and more explicit than SAPRC; however both approaches are acceptable within the current state of the science.

For benzene the product yields of many species are different between the mechanisms, especially for HO_2 but it is difficult to determine which approach is better given the complex nature of aromatic oxidation.

Methyl Peroxy Radical Reactions

The reaction rate parameter for the reaction of methyl peroxy radical with nitric oxide of SAPRC-07 has a somewhat different temperature dependence than

CB05 and RACM2. Also the rate constant for the reaction, $\text{MEO}_2 + \text{HO}_2 \rightarrow \text{HCHO}$, may be too high.

SAPRC-07 has a superior treatment of the self-reaction of the methyl peroxy radical that allows the temperature dependence of the branching ratio to be simulated.

t-Butoxy Radical Reactions

SAPRC-07 alone includes a direct treatment of t-butoxy radical reactions. This should help it more accurately account for the yield of organic nitrate and it might help it characterize secondary organic aerosol yields.

Peroxy Radical Operators

SAPRC-07 has its own scheme of using operators to treat peroxy radical reactions. SAPRC-07 includes a number of active peroxy radical operators and it uses the operator approach much more extensively than either CB05 or RACM2. SAPRC's approach to the treatment of peroxy radical chemistry this level of treatment is very reasonable. The SAPRC-07 operator scheme is within the state of the science.

Reactions Involving PAN, Homologues and Acyl Peroxy Radicals

SAPRC-07 includes a higher peroxyacetyl nitrate compound and an aromatic PAN like compound that are not included in CB05 and RACM2. This is a good feature because when mechanisms are simplified, much of the carbon is channeled to acetaldehyde and formaldehyde much faster than in reality. Having more of the higher aldehydes and peroxyacetyl nitrate compounds helps reduce this problem.

PAN Homologue from Methacrolein and Peroxy Radicals from Acroleins

SAPRC-07 includes the photolysis of the PAN homologue. Overall, it seems advisable to characterize the formation of this peroxyacetyl nitrate even though biological emissions are usually most important in regions with lower NO_x .

Formaldehyde Reactions

The reaction $\text{HCHO} + \text{HO}_2 \rightarrow \text{HOCOO} + \text{H}_2$ and subsequent reactions for HOCOO could be eliminated to save computational resources. Sensitivity tests made during the development of RACM2 for realistic atmospheric conditions showed that this reaction was not significant.

Acetaldehyde Reactions and Higher Aldehyde Reactions

The three mechanisms treat this chemistry very similarly. The only significant differences are the products produced by higher aldehydes in their photolysis reactions and by their reaction with HO. SAPRC-07 produces several operator radicals while CB05 produces one operator radical and RACM2 produces a surrogate radical species. The SAPRC-07 approach may allow better treatment of some compounds that are aggregated into the RCHO species.

Acetone Reactions and Ketone Reactions

CB05 does not include acetone and other ketones as separate species rather it includes a species for isoprene products representing methyl vinyl ketone and methacrolein. Given acetone's importance as a radical source at higher altitudes in the troposphere this makes CB05 unsuited for large spatial scale models that need to model the upper troposphere. SAPRC-07 and CB05 differ in their treatment of products. SAPRC-07 produces a large number of operator radicals while RACM2 produces surrogate radical species that participate in the reactions listed for RACM2 in this section. The differing SAPRC-07 and RACM2 methods should lead to similar simulations.

Dicarbonyl Reactions

There are three photolysis reactions of glyoxal: a reaction that produces HO₂ and CO; a reaction that produces HCHO and CO; and a third reaction that produces H₂ and CO. RACM2 includes all three but SAPRC-07 omits the third. Another concern is that for the reactions of glyoxal with HO and nitrate radical SAPRC-07 forms a higher acyl peroxy radical and a negative quantity of lost carbon. This seems surprising; it is very unclear what purpose this serves. This appears to offset the production of the higher acyl peroxy radical but does subtracting lost carbon add carbon to the system?

Methacrolein, Methyl Vinyl Ketone and Isoprene Products

The products of the reaction of methacrolein with HO, O₃ and NO₃ are very different between the three mechanisms. SAPRC-07 includes reactions for a species that represents lumped isoprene products that is not equivalent to the treatment in the other two mechanisms.

Methanol, Organic Acid and Organic Peroxide Reactions

The three mechanisms compared (SAPRC, CB05 and RACM2) treat this chemistry very similarly. The treatment of acetic acid could be improved in SAPRC-07.

SAPRC-07 includes the reactions of lumped organic peroxides with greater than 5 carbon atoms with HO and its photolysis reactions. This may provide some advantage for SAPRC-07 in the modeling of aqueous phase chemistry.

SAPRC-07 Chlorine Reactions

SAPRC-07 is the only one of the mechanisms with chlorine chemistry in the versions that were examined. SAPRC-07 includes the major inorganic reactions of chlorine and the reactions of chlorine atom with organic compounds. The reactions of chlorine are within the state of the science.

Chapter 2. Comparison of Chemical Species in the Mechanisms

Species by Species Comparison

SAPRC-07 and RACM2 share a more explicit, aggregated molecule approach. Similar organic compounds are aggregated into the same model species. CB05 was originally based on species that reflected the concentrations of organic functional groups in a given air sample but it has evolved become closer to the aggregated molecular approach used in SAPRC-07 and RACM2.

SAPRC-07 and RACM2 are more explicit than CB05 in their “constant” species, species that are unchanged by chemical reactions. SAPRC-07 includes the overall concentration of air and oxygen while RACM2 includes oxygen and nitrogen. This is a difference without distinction. It is an advantage of SAPRC-07 over CB05 because none of the constant species are included in CB05.

All three mechanisms have eleven active inorganic species in common such as NO, NO₂, O₃, etc along with HO and HO₂ radicals and ground state and excited state oxygen atoms. This number of species is consistent with the relatively explicit treatment of atmospheric inorganic chemistry in the models. In addition SAPRC-07 includes another six active inorganic species that contain chlorine and the reactive intermediates, chlorine atom and ClO. The treatment of the reaction of hydroxyl radical with hydrochloric acid is correct in the gas-phase.

SAPRC-07 and RACM2 both include the primary reactions of methane, ethane, isoprene, acetylene and benzene but CB05 does not explicitly include acetylene and benzene. CB05 and RACM2 treat ethane explicitly while SAPRC-07 uses an aggregated species, ALK1. CB05 remains closest to its roots in its treatment of alkanes. PAR represents remains a “paraffin carbon bond” that treats the reactions of –CH₂– groups without consideration of the specific molecule in which it is found. SAPRC-07 includes a range of aggregated alkane species, ALK1, ALK2, ALK3, ALK4 and ALK5. Alkanes are aggregated into these species according to their rate constants with the hydroxy radical. ALK1 is mostly ethane, ALK2 is mostly propane while ALK3, ALK4 and ALK5 are mixtures of a number of alkanes. RACM2 uses a similar approach but SAPRC-07 has one more aggregated alkane species. Aerosol yields depend on the molecular weight of the reacting alkane. The SAPRC-07 approach is superior for treatment of the aerosol formation from alkanes because it retains some carbon number information while this is explicitly not treated in CB05.

The three mechanisms have very different reaction schemes for aromatics although SAPRC-07 and CB05 have two initial species and RACM2 has three. In SAPRC-07 the species ARO1 and ARO2 represent lower and higher reactive aromatics based on their rate constants with hydroxyl radical. CB05 aggregates aromatics into a species representing toluene and other monoalkyl aromatic compounds and a second species that represents xylene and other polyalkyl

aromatics compounds. RACM2 is similar but it divides xylene and other polyalkyl aromatics onto a species for meta- and para-polyalkyl aromatics and another for the ortho-polyalkyl aromatics. The RACM2 extra species allows more direct comparison of simulations with most field measurement data, for example, m-xylene and p-xylene will co-elute on gas chromatograph while o-xylene has no such co-elution problems. It is much more difficult to measure all three isomers by gas-chromatography (although this is done in a small number of laboratories). The number of initial aromatics in SAPRC-07 is adequate for air quality modeling given the present state of knowledge.

The species used to represent alkenes in the three mechanisms is somewhat analogous to those used to treat aromatics. SAPRC-07 has two alkene species OLE1 and OLE2 represent lower and higher reactive alkenes based on their rate constants with hydroxyl radical. CB05 and RACM2 aggregate alkenes into a species representing those compounds with the double bond at the end of a molecule and another species with the double bond within the molecule. RACM2 also includes a diene species to account for anthropogenic dienes. The SAPRC-07 approach is better in capturing the initial reactivity of a reacting mixture while the CB05 and RACM2 approach in principle would be more faithful to reproducing the secondary products.

All three mechanisms include the biogenically emitted species, isoprene. SAPRC-07 and CB05 include a single species for terpenes, TERP, and RACM2 includes two, one for Alpha-pinene and similar compounds, API, and d-limonene and similar compounds, LIM. The oxidation of isoprene in SAPRC-07 is the same as in SAPRC99 and it includes species for methacrolein, methyl vinyl ketone and one for other isoprene products. RACM2 includes methacrolein and methyl vinyl ketone while CB05 includes only ISPD, isoprene products. Given the large number of biogenically emitted species it is probably true that none of the mechanisms include sufficient detail to accurately model the effects of these compounds on air quality (Fuentes et al, 2000).

The mechanisms are very different in their treatment of peroxy radicals. The extensive steady-state operator approach used by SAPRC-07 is one of its most distinguishing features. It reduces the number of species and reactions in the mechanism. It helps the mechanism to adequately account for the number of NO to NO_2 conversions caused by peroxy reactions with nitric oxide. SAPRC-07's operator approach also allows the formation of organic peroxides to be calculated. CB05 uses fewer operators, XO_2 for NO to NO_2 conversions and XO_2N for NO to organic nitrate conversions. RACM2 uses a more explicit approach for the representation of peroxy radical reactions. The three mechanisms include methyl peroxy radical, acetyl peroxy radical and higher acyl peroxy radical, although RACM2 specifies that the corresponding radical is saturated. The explicit treatment of the acetyl peroxy and acyl peroxy radicals underscores the importance of PAN and its higher homologs. SAPRC-07 includes an aromatic aldehyde peroxy radical while RACM2 includes three

peroxy radicals formed from benzaldehyde. SAPRC-07 includes a peroxy radical formed from acroleins while RACM2 includes several peroxy radicals formed from methacrolein. CB05 and RACM2 include a toluene-hydroxyl radical adduct and an aromatic ring opening products while SAPRC-07 uses another approach to aromatic chemistry. RACM2 uses several more species to represent toluene-hydroxyl peroxy radicals and their products than either SAPRC-07 or RACM2.

SAPRC's treatment of peroxy-radicals is well thought-out and Dr. Carter is to be commended for its construction. The fractions of peroxy radical that react with nitric oxide, another peroxy radical, nitrate radical or another species and the products depends on the NO_x/VOC ratio and the overall pollution levels. This is accounted for SAPRC-07 in contrast to CB05. CB05 using a weaker operator approach assigns most of the mass of the secondary products to the species formed from the peroxy radical-nitric oxide reaction only. This is an adequate approach for highly and moderately polluted regions but it becomes less accurate on the regional scale where the concentrations of nitrogen oxides become lower. Clearly SAPRC-07 is superior to CB05 in this respect.

The three mechanisms include three aldehydes: formaldehyde, acetaldehyde and propanal (and higher). SAPRC-07 and RACM2 treat acetone and methyl ethyl ketone while CB05 does not include treatment of ketones. SAPRC-07 includes an additional species to describe fast reacting ketones. Given that acetone is a major radical source in the upper troposphere this is an important advantage of SAPRC-07 and RACM2 over CB05 for modeling over larger spatial scales. RACM2 includes further detailed treatment of ketones, including species for higher ketones, hydroxyacetone (and other C₃ ketones) and hydroxy ketone. SAPRC-07 and RACM2 have glyoxal and methyl glyoxal as dicarbonyl species. CM05 omits glyoxal while SAPRC-07 also includes biacetyl. The treatment of carbonyl compounds appears to be reasonable.

RACM2 has a more detailed treatment of alcohols, it includes methanol, ethanol and propanol (and higher alcohols). RACM2 also includes ethylene glycol. SAPRC-07 explicitly includes methanol and aggregates ethanol while CB05 includes methanol and ethanol. Alcohols may have some significance in affecting reactivity under relatively clean conditions. Some thought should be given to adding more detail to SAPRC-07's treatment of alcohols when it is used at larger spatial scales.

All three mechanisms include a species for organic nitrates but RACM2 includes an additional species to include nitro-oxyacetaldehyde. SAPRC-07 is superior to CB05 in that it includes four species for peroxy acetyl nitrates: one for peroxyacetyl nitrate (PAN), one for propyl-peroxyacetyl nitrate (PPN and higher), one for aldehyde aromatic PANs (PBZN) and a species for the PAN homolog formed from methacrolein (MAPAN). RACM2 does not include a species for aldehyde aromatic PANs while CB05 has only PAN and PPN.

All three mechanisms include species for formic acid, acetic acid and higher peroxy carboxylic acids. SAPRC-07 has one additional species for higher organic acids. RACM2 and CB05 aggregate higher acids with acetic acid and higher peroxy carboxylic acids with peroxyacetic acid. SAPRC-07 has greater detail in species for organic peroxides. All three mechanisms include methyl hydrogen peroxide. CB05 and RACM2 have a higher organic peroxide species while SAPRC-07 contains four other species to describe peroxides: one for lumped ROOH with 2 to 4 carbon atoms, one for lumped ROOH with ≥ 5 carbon atoms, a ROOH species formed due to HO addition to aromatics for secondary organic aerosol formation and another to represent the photolysis of ROOH. These SAPRC-07 organic peroxides are more of operator species than real species.

Aromatic oxidation results in a large number of secondary organic products. SAPRC-07 includes a reasonable number of species to describe the oxidation of organic compounds. In contrast CB05 includes only cresol. The SAPRC-07 species include one for chenols and cresols, one for nitrophenols, one for aromatic aldehydes and three unsaturated ring fragmentation products. The species in RACM2 is similar to those in CB05: one for cresol and similar compounds, one for phenol, one for methyl catechol, one for benzaldehyde and other aromatic aldehydes and three species to represent unsaturated dicarbonyls that correspond somewhat to SAPRC-07's unsaturated ring fragmentation products.

The treatment of chlorine in a standard version of the mechanism is unique to SAPRC-07. SAPRC-07 includes the two most important chlorinated atmospheric organic compounds chloroacetaldehyde and chloroacetone.

Table 2-1. Comparison of Species in the Mechanisms SAPRC-07 – CB05 – RACM2

SAPRC		CB05		RACM2	
Constant Species					
			N2	nitrogen	
O2	oxygen		O2	oxygen	
M	air				
H2O	water		H2O	water	
H2	hydrogen molecule		H2	hydrogen	
HV	light		HV	light	
Active Inorganic Species					
O3	ozone	O3	ozone	O3	ozone
NO	nitric oxide	NO	nitric oxide	NO	nitric oxide
NO2	nitrogen dioxide	NO2	nitrogen dioxide	NO2	nitrogen dioxide
NO3	nitrate radical	NO3	nitrate radical	NO3	nitrogen trioxide
N2O5	nitrogen pentoxide	N2O5	dinitrogen pentoxide	N2O5	dinitrogen pentoxide
HONO	nitrous acid	HONO	nitrous acid	HONO	nitrous acid
HNO3	nitric acid	HNO3	nitric acid	HNO3	nitric acid
HNO4	peroxynitric acid	PNA	peroxynitric acid	HNO4	pernitric acid
HO2H	hydrogen peroxide	H2O2	hydrogen peroxide	H2O2	hydrogen peroxide
CO	carbon monoxide	CO	carbon monoxide	CO	carbon monoxide
SO2	sulfur dioxide	SO2	sulfur dioxide	SO2	sulfur dioxide
Active Radical Species					
OH	hydroxyl radical	OH	hydroxyl radical	HO	hydroxy radical
HO2	hydroperoxide radical	HO2	hydroperoxy radical	HO2	hydroperoxy radical
MEO2	methyl peroxy radical	MEO2	methyl peroxy radical	MO2	methyl peroxy radical
				ETHP	peroxy radicals formed from ETH
				HC3P	peroxy radicals formed from HC3

Table 2-1, Continued. Comparison of Species in the Mechanisms SAPRC-07 – CB05 – RACM2

				HC5P	peroxy radicals formed from HC5
				HC8P	peroxy radicals formed from HC8
				ETEP	peroxy radicals formed from ETE
				OLTP	peroxy radicals formed from OLT
				OLIP	peroxy radicals formed from OLI
				OLND	NO3-alkene adduct reacting via decomposition
				OLNN	NO3-alkene adduct reacting to form carbonitrates + HO2
				ACTP	peroxy radicals formed from ACT
				KETP	peroxy radicals formed from KET
				MEKP	peroxy radicals formed from MEK
				UALP	peroxy radicals formed from UALD
		TO2	toluene-hydroxyl radical adduct	TOLP	peroxy radicals formed from TOL
		OPEN	aromatic ring opening product	TLP1	peroxy radicals formed from TOL
				TR2	peroxy radicals formed from TOL
				PER1	peroxy intermediate formed from TOL
				PER2	peroxy intermediate formed from TOL
				XYLP	peroxy radicals formed from XYL
				XYL1	peroxy radicals formed from XYL

Table 2-1, Continued. Comparison of Species in the Mechanisms SAPRC-07 – CB05 – RACM2

				XY2	peroxy radicals formed from XYL
				XYO2	peroxy radicals formed from XYO
				XYOP	peroxy radicals formed from XYO
				ADDC	aromatic-HO adduct from CSL
				ADCN	nitrate-peroxy aromatic-HO adduct formed from CSL + NO ₃
				ADDP	aromatic-HO adduct from PHEN
				ISHP	beta-hydroxy hydroperoxides from ISOP+HO ₂
				ISON	beta-hydroxyalkylnitrates from ISOP+NO; alkylnitrates from ISO+NO ₃
MACO3	peroxy radical from acroleins			MACP	peroxy radicals formed from MACR+HO
				MAHP	hydroperoxides from MACP+HO ₂
				MVKP	peroxy radicals formed from MVK
				LIMP	peroxy radicals formed from LIM
MECO3	acetyl peroxy radical	C2O ₃	acetyl peroxy radical	ACO3	acetyl peroxy radical
				ORAP	peroxy radical from ORA2
RCO3	higher acyl peroxy radical	CXO ₃	higher acyl peroxy radical	RCO3	higher saturated acyl peroxy radicals
BZCO3	aromatic aldehyde peroxy radical			BALP	peroxy radicals formed from BALD

Table 2-1, Continued. Comparison of Species in the Mechanisms SAPRC-07 – CB05 – RACM2

			BAL1	peroxy radicals formed from BALD
			BAL2	peroxy radicals formed from BALD

SAPRC		CB05			RACM2
Active Peroxy Radical Operators					
RO2C	NO to NO ₂ and NO ₃ to NO ₂ conv.	XO ₂	NO to NO ₂ conversion	XO ₂	Accounts for addition NO to NO ₂ conversions
RO2XC	NO consumption				
RO2R	NO to NO ₂ conv. with HO ₂ form.				
R2O ₂	NO to NO ₂ conv. w/o HO ₂ form.				
RO2N	NO consmp. w ONIT form.	XO _{2N}	NO to ONIT conversion		
Steady State Radical Species					
O3P	Ground State Oxygen Atom	O	O ₃ (P) Oxygen atom	O3P	Ground state oxygen
O1D	Excited Oxygen Atoms	O1D	O1(D) Oxygen atom	O1D	Excited oxygen atom
		ROR	Secondary alkoxy radical		
TBUO	t-Butoxy Radicals				
BZO	Phenoxy Radicals	CRO	Methylphenoxy radical	PHO	Phenoxy radical formed from phenol
				CHO	Phenoxy radical formed from CSL

				BENP	Peroxy radicals formed from BEN
				MCTO	Phenoxy radical from Methyl Catechol
				MCTP	Peroxy radicals formed from MCTO + O ₃
HOCOO	Radical from HCHO + HO ₂	HCO3	Radical from HCHO + HO ₂		
PAN and PAN Homologues					
PAN	Peroxy Acetyl Nitrate	PAN	Peroxyacetyl nitrate	PAN	Peroxyacetyl nitrate
PAN2	PPN and higher alkyl PANs	PANX	C3 and higher PANs	PPN	Peroxypropionyl nitrate and higher
PBZN	Aldehyde Aromatic PANs				
MAPAN	PAN from Methacrolein			MPAN	PAN from Methacrolein

Table 2-1, Continued. Comparison of Species in the Mechanisms SAPRC-07 – CB05 – RACM2

Explicit & Lumped React. Organic Products					
HCHO	Formaldehyde	FORM	Formaldehyde	HCHO	Formaldehyde
CCHO	Acetaldehyde	ALD2	Acetaldehyde	ACD	Acetaldehyde
RCHO	Lumped C3+ Aldehydes	ALDX	Propionaldehyde & higher	ALD	≥C3 aldehydes
ACET	Acetone			ACT	Acetone
MEK	Ketones & other oxygenated			MEK	Methyl ethyl ketone
				KET	Higher Ketones
				HACE	Hydroxyacetone and other C3 ketones
				HKET	Hydroxy ketone

MEOH	Methanol	MEOH	Methanol	MOH	Methanol
		ETOH	Ethanol	EOH	Ethanol
				ROH	C3 and higher alcohols
				ETEG	Ethylene glycol
FACD	Formic Acid	FACD	Formic acid	ORA1	Formic acid

SAPRC		CB05		RACM2	
Explicit & Lumped React. Organic Products					
CCOOH	Acetic Acid	AACD	Acetic and higher RCOOH	ORA2	Acetic acid and higher
RCOOH	Higher RCOOH				
PACD	Peroxyacetic and higher peroxycarboxylic acids	PACD	Peroxyacetic and higher peroxycarboxylic acids	PAA	Peroxyacetic acid and higher analogs
COOH	Methyl Hydroperoxide	MEPX	Methylhydroperoxide	OP1	Methyl hydrogen peroxide
ROOH	Lumped ROOH with 2-4 Carbons	ROOH	Higher organic peroxide	OP2	Higher organic peroxides
R6OOH	Lumped ROOH with ≥ 5 Carbons				
RAOOH	ROOH due to OH addition to aromatics for SOA formation				
XOOH	Represents photolysis of ROOH				
Dicarbonyls					
GLY	Glyoxal			GLY	Glyoxal
MGLY	Methyl Glyoxal	MGLY	Methyl Glyoxal and other aromatic products	MGLY	Methylglyoxal and other α -carbonyl aldehydes

Table 2-1, Continued. Comparison of Species in the Mechanisms SAPRC-07 – CB05 – RACM2

BACL	Biacetyl				
Aromatic Products					
CRES	Phenols and Cresols	CRES	Cresols	CSL	Cresol and similar
				PHEN	Phenol
				MCT	Methyl Catechol
NPHE	Nitrophenols				
BALD	Aromatic aldehydes			BALD	Benzaldehyde and other aromatic aldehydes
MACR	Methacrolein	ISPD	Isoprene Products	MACR	methacrolein
MVK	Methyl Vinyl Ketone	ISPD	Isoprene Products	MVK	Methyl vinyl ketone
IPRD	Lumped isoprene products	ISPD	Isoprene Products		
Aromatic unsaturated ring fragm. products					
AFG1	Photolyze to form radicals			DCB1	Unsaturated dicarbonyls
AFG2	photolyze to form non-radicals			DCB2	Unsaturated dicarbonyls
AFG3	Lumped diunsaturated dicarbonyl			DCB3	Unsaturated dicarbonyls
				UALD	Unsaturated aldehydes
				EPX	Epoxide formed in TOL, XYL and XYO reactions
Lumped Parameter Products					
PROD2	Fast reacting Ketones				
RNO3	Lumped Organic Nitrates	NTR	Organic nitrate	ONIT	Organic nitrate
				NALD	nitro-oxyacetaldehyde

SAPRC		CB05		RACM2	
	Steady state operators used to represent radical or product formation in peroxy radical reactions				
xHO2	Formation of HO2 from alkoxy radicals formed in peroxy radical reactions with NO and NO3 (100% yields) and RO2 (50% yields)				

Table 2-1, Continued. Comparison of Species in the Mechanisms SAPRC-07 – CB05 – RACM2

xOH	As above except for OH.				
xNO2	Ditto				
xMEO2	Ditto				
xMECO3	Ditto				
xRCO3	Ditto				
xMACO3	Ditto				
xTBUO	Ditto				
xCO	Ditto				
xHCHO	Ditto				
xCCHO	Ditto				
xRCHO	Ditto				
xACET	Ditto				
xMEK	Ditto				
xPROD2	Ditto				
xGLY	Ditto				
xMGLY	Ditto				
xBACL	Ditto				
xBALD	Ditto				
xAFG1	Ditto				
xAFG2	Ditto				
xAFG3	Ditto				
xMACR	Ditto				

SAPRC		CB05		RACM2	
Steady state operators used to represent radical or product formation in peroxy radical reactions – Continued					
xMVK	Ditto				
xIPRD	Ditto			ISOP	Peroxy radicals formed from ISO+HO
				APIP	Peroxy radicals formed from API
xRNO3	Ditto				
zRNO3	Formation RNO3 in RO2 + NO				
yROOH	Formation ROOH after RO2+HO2				

Table 2-1, Continued. Comparison of Species in the Mechanisms SAPRC-07 – CB05 – RACM2

yR6OOH	Ditto				
yRAOOH	Ditto				
Non-Reacting Species					
CO2	Carbon Dioxide			CO2	Carbon dioxide
SULF	Sulfates (SO3 or H2SO4)	SULF	Sulfuric acid (g)	SULF	Sulfuric acid
XC	Lost Carbon or unreactive carbon				
XN	Lost Nitrogen or unreactive				
Primary Organics Represented Explicitly					
CH4	Methane	CH4	Methane	CH4	Methane
ETHE	Ethene	ETH	Ethene	ETE	Ethene
ISOP	Isoprene	ISOP	Isoprene	ISO	Isoprene
ACYE	Acetylene			ACE	Acetylene
BENZ	Benzene			BEN	Benzene
Lumped model emitted VOC					
ALK1	Primarily ethane	ETHA	Ethane	ETH	ethane
ALK2	Primarily propane	PAR	Paraffin carbon bond	HC3	$k_{HO} < 3.4 \times 10^{-12} \text{ cm}^3 \text{ s}^{-1}$
ALK3	Alkanes with k_{OH} between 2.5×10^3 and $5 \times 10^3 \text{ ppm}^{-1} \text{ min}^{-1}$	PAR	Paraffin carbon bond	HC5	k_{HO} between 3.4×10^{-12} to $6.8 \times 10^{-12} \text{ cm}^3 \text{ s}^{-1}$

SAPRC		CB05		RACM2	
Lumped model emitted VOC					
ALK4	Alkanes with k_{OH} between 5×10^3 and $1 \times 10^4 \text{ ppm}^{-1} \text{ min}^{-1}$	PAR	Paraffin carbon bond		
ALK5	Alkanes with k_{OH} greater than $1 \times 10^4 \text{ ppm}^{-1} \text{ min}^{-1}$	PAR	Paraffin carbon bond	HC8	$k_{OH} > 6.8 \times 10^{-12} \text{ cm}^3 \text{ s}^{-1}$

Table 2-1, Continued. Comparison of Species in the Mechanisms SAPRC-07 – CB05 – RACM2

ARO1	Aromatics with kOH <2x10 ⁴ ppm ⁻¹ min ⁻¹	TOL	Toluene & other monoalkyl aromatics	TOL	Toluene and less reactive aromatics
ARO2	Aromatics with kOH >2x10 ⁴ ppm ⁻¹ min ⁻¹	XYL	Xylene & other polyalkyl aromatics	XYL	m, p-xylene
				XYO	o-xylene
OLE1	Alkenes with kOH < 7x10 ⁴ ppm ⁻¹ min ⁻¹	OLE	Terminal olefin carbon bond	OLT	Terminal alkenes
OLE2	Alkenes with kOH > 7x10 ⁴ ppm ⁻¹ min ⁻¹	IOLE	Internal olefin carbon bond	OLI	Internal alkenes
				DIEN	Butadiene and other anthropogenic dienes
TERP	Terpenes	TERP	Terpene	API	Alpha-pinenes and similar
				LIM	d-limonene and similar

Table 2-1, Continued. Comparison of Species in the Mechanisms SAPRC-07 – CB05 – RACM2

SAPRC-07 Chlorine Species

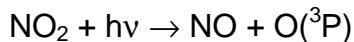
SAPRC					
Active Inorganic Species					
CL2	Chlorine molecules				
CLNO	CINO				
CLONO	CIONO				
CLNO2	CINO ₂				
CLONO2	CIONO ₂				
HOCL	HOCl				
Active Chlorine Radical Species					
CL	Chlorine atom				
CLO	CIO Radical				

SAPRC					
Steady State Operators					
xCL	Formation of Cl radicals from alkoxy radicals formed in peroxy radical reactions with NO and NO ₃ and RO ₂				
RO ₂ CL	Represents NO to NO ₂ conversion with Cl formation				
xCLCCHO	As above, but for CLCCHO				
xCLACET	As above, but for CLACET				
Active Organic Product Species					
CLCCHO	Chloroacetaldehyde				
CLACET	Chloroacetone				
Low Reactivity Compounds					
HCL	Hydrochloric acid				
CLCHO	Formyl Chloride				
Testing Purposes Only					
CHCl ₃	Chloroform				

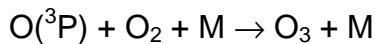
Chapter 3. Comparison of Chemical Reactions in the Mechanisms

Inorganic Reactions

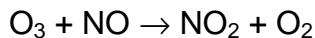
The inorganic chemistry that an air quality chemical mechanism must describe is relatively understood well. Tropospheric ozone is formed by the photolysis of nitrogen dioxide to produce nitric oxide and ground state oxygen atoms.



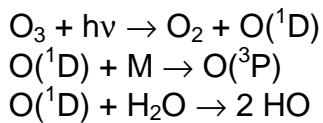
The oxygen atoms react with molecular oxygen to produce ozone. The species M represents a molecule of nitrogen, oxygen or other species that is required to remove excess energy so that that ozone molecule may be stabilized.



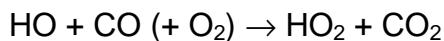
Ozone may react with nitric oxide to reproduce nitrogen dioxide.



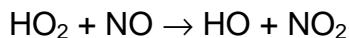
Ozone photolysis reactions may lead to the production of O(¹D), an energetically excited oxygen atom, with sufficiently energetic photons. Most of the O(¹D) are quenched back to the ground state O(³P) that immediately react with oxygen to reproduce ozone. A few percent live long enough to react with water vapor to form the hydroxyl radical.



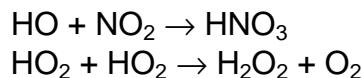
The hydroxyl radical reacts with carbon monoxide and many organic species to produce peroxy radicals. The reaction of HO with CO illustrates the formation of the hydroperoxy radical by the reaction of the hydroxyl radical with carbon monoxide.



The formation of the hydroperoxy radical provides a key pathway to the “extra” conversions of nitric oxide to nitrogen dioxide that are needed for ozone production.



The photolysis of nitrogen dioxide will reform nitric oxide and the hydroxyl radical can react again to produce more hydroperoxy radicals. This cycling between HO and HO₂ and between NO and NO₂ are examples of chain reactions. Chain reactions must terminate and there are two particularly important chain-terminating reactions in the troposphere. Reaction of HO with NO₂ leads to the formation of nitric acid and the self-reaction of HO₂ leads to the formation of hydrogen peroxide.



Note that the overall rate parameter for the self-reaction of HO₂ depends on atmospheric pressure and the water vapor concentration (Stockwell, 1995). The reaction of HO with NO₂ is more important for urban conditions where nitric oxide concentrations are high while the self-reaction of HO₂ is more important for more remote conditions where nitric oxide concentrations are low.

All three mechanisms incorporate these basic inorganic reactions but there are some differences. The most significant are discussed below.

The rate constant of the O₃ + NO reaction in SAPRC-07 and CB05 is different than RACM2. At 300 K the rate constant of SAPRC-07 is greater than RACM2 by 14%. This will have some effect on the ozone destruction rate.

SAPRC-07 and RACM2 include the reaction of O³P + O₃ but CB05 does not. This will have little effect on ozone at the surface level but this reaction can be more important near the tropopause.

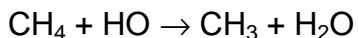
SAPRC-07 and CB05 include the third order reaction, N₂O₅ + H₂O + H₂O → 2*HNO₃ but RACM2 does not. This reaction is a reasonable addition. At a temperature of 298 K, 1 atmosphere and 100% relative humidity this reaction yields a lifetime of N₂O₅ that is a little less than a half hour. At the same temperature and pressure at 75%, 50% and 10% the lifetime of N₂O₅ will be 0.45 hour, 1 hour and 1 day, respectively.

The quenching reaction of O¹D with the background atmosphere is an important process that affects the concentration of hydroxyl radical. SAPRC-07 has a single reaction, O¹D + M, with a single rate parameter. RACM2 includes two reactions, one for the quenching reaction of N₂ and another for O₂. There is some difference in the activation energies for the two reactions and therefore including two reactions allows the altitude dependence of quenching of O¹D to be better simulated.

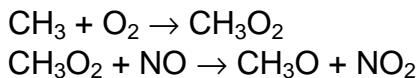
The activation energy for the HO₂ + O₃ → HO + O₂ in SAPRC-07 is inconsistent with the cited reference.

Methyl Peroxy Radical Reactions

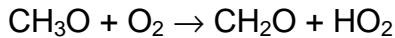
The reaction of the hydroxyl radical with organic compounds leads to the production of hydroperoxy radicals and a wide variety of organic peroxy radicals. Methane is the simplest organic compound. Methane reacts with the hydroxyl radical where the HO abstracts a hydrogen atom to form a methyl radical and water.



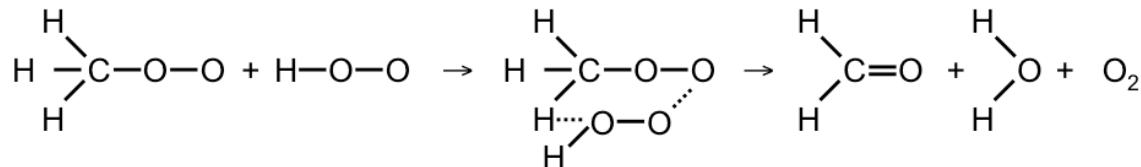
The methyl radical rapidly reacts with oxygen to produce a methyl peroxy radical that may react with nitric oxide to produce a methyoxy radical and nitrogen dioxide.



The methyoxy radical reacts with oxygen to form formaldehyde and a hydroperoxy radical.



The reaction rate parameter for the reaction of methyl peroxy radical with nitric oxide of SAPRC-07 has a some-what different temperature dependence than CB05 and RACM2. Also the reaction: $\text{MEO}_2 + \text{HO}_2 \rightarrow \text{HCHO}$ seems surprising. Does the reaction involve the formation of water and a cyclic intermediate as shown below?



If it does involve an intermediate as above, is the SAPRC-07 rate constant too high? The formation of the cyclic intermediate would seem have a lower probability due to entropy considerations.

SAPRC-07 and RACM2 include the reaction of NO_3 with the methyl peroxy radical but CB05 does not. CB05 will be less accurate in regions where the NO_x levels are intermediate such as in suburban areas.

SAPRC-07 includes two reactions for the self-reaction of the methyl peroxy radical; one for the methyoxy radical pathway and the other for the hydrogen-shift pathway. This approach allows the branching ratio to adjust to temperature since

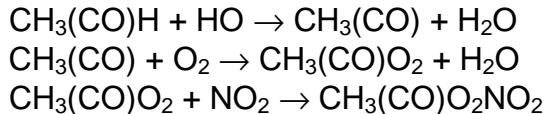
the two reactions have different activation energies. This is unique to SAPRC-07.

RO2C and Other Active Peroxy Radical Operators

SAPRC-07 includes a number of active peroxy radical operators and it uses the operator approach much more extensively than either CB05 or RACM2. CB05 has one operator, XO₂, which reacts with NO and few other radical species. SAPRC's active peroxy radical operators react with NO, HO₂, CH₃O₂, NO₃ and themselves (self reaction). RACM2 includes one similar species, XO₂ that reacts similar to the SAPRC-07 active peroxy radical operator species. RACM2's XO₂ reactions are listed for comparison under SAPRC's RO2C reactions. Given SAPRC's approach to the treatment of peroxy radical chemistry this level of treatment is very reasonable and within the state of the science.

Reactions Involving PAN, Homologues and Acyl Peroxy Radicals

Peroxyacetyl nitrate, CH₃(CO)O₂NO₂, (PAN) is a very important chemical species produced from acetaldehyde and nitrogen dioxide. The mechanism of PAN formation begins with the abstraction of the aldehylic hydrogen atom by the hydroxyl radical and the addition of oxygen to the CH₃(CO) radical.



Nitrogen dioxide will add to the CH₃(CO)O₂ to produce PAN. Note that at temperatures near 25 °C PAN is in equilibrium with nitrogen dioxide and the CH₃(CO)O₂ radical but at colder temperatures PAN is much more stable.

The three mechanisms include PAN formation, its thermal decomposition and its photolysis. All three mechanisms include reactions of the acetyl peroxy radical with NO, HO₂, CH₃O₂, its self-reaction and with operator radicals. The three mechanisms include PPN formation and treat it similarly to PAN except RACM2 does not include its photolysis. SAPRC-07 includes a higher peroxyacetyl nitrate compound and an aromatic PAN-like compound that are not included in CB05 and RACM2. This is a good feature because when mechanisms are simplified, much of the carbon is channeled to acetaldehyde and formaldehyde much faster than in reality. Having more of the higher aldehydes and peroxyacetyl nitrate compounds helps reduce this problem.

PAN Homologue from Methacrolein and Peroxy Radicals from Acroleins

The oxidation of isoprene and other biogenically emitted VOC produces PAN homologues. To account for these processes, SAPRC-07 and RACM2 form a peroxyacetyl nitrate compound from the acyl radical produced by methacrolein

oxidation. This compound is not formed in CB05. Both SAPRC-07 and RACM2 treat the acyl radical produced from methacrolein similar to the way they each treat active peroxy radical operators. The major difference between SAPRC-07 and RACM2 is that SAPRC-07 includes this PAN's photolysis while RACM2 does not. This is a virtue for SAPRC-07. Overall, it seems advisable to characterize the formation of this peroxyacetyl nitrate even though biological emissions are usually most important in regions with lower NO_x. This would be due to the PAN's greater relative effect on NO_x concentrations.

t-Butoxy Radical Reactions

SAPRC-07 alone includes a direct treatment of t-butoxy radical reactions. This should help it more accurately account for the yield of organic nitrate and it might help it characterize secondary organic aerosol yields.

Phenoxy Radicals

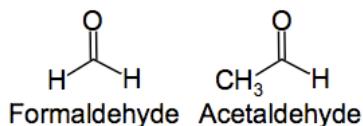
Atmospheric aromatic chemistry remains very difficult to characterize due to its complexity and its many remaining scientific uncertainties. The divergence between the mechanisms is great and therefore it is difficult to align their reactions. All three include phenoxy radical species that react with NO₂ and HO₂. SAPRC-07 and CB05 have a direct decomposition pathway to form cresol but RACM2 does not.

Steady State Operators for Representing Radical or Product Formation in Peroxy Radical Reactions

It is necessary to reduce the numbers of peroxy radical reactions because of the extremely large number of potential reactions. SAPRC-07 has its own scheme of using operators to treat peroxy radical reactions. CB05 uses a very highly simplified scheme while RACM2 uses a much more explicit treatment of peroxy radical reactions that is limited to the classes of reactions that have been demonstrated to be most important. The number of operator species seems to be great enough to support a reasonable level of accuracy. The SAPRC-07 operator scheme is within the state of the science.

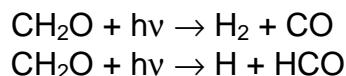
Formaldehyde Reactions

Formaldehyde is the simplest aldehyde (CH₂O) and acetaldehyde (CH₃CHO) is the next most complex, these compounds are shown below.

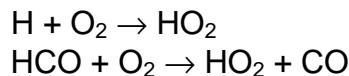


The photolysis of formaldehyde is a radical source that in some polluted urban regions may be as important as ozone. There are two atmospherically important

photolysis reactions for formaldehyde; one reaction produces molecular hydrogen and carbon monoxide and the other reaction produces hydrogen atoms and the CHO radical.



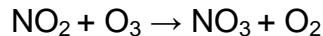
Following the photolysis of formaldehyde the hydrogen atom and the HCO radical react with oxygen to produce hydroperoxy radicals.



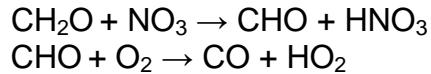
The three mechanisms use the same reactions for formaldehyde except that SAPRC-07 and CB05 include the reaction $\text{HCHO} + \text{HO}_2 \rightarrow \text{HOCOO} + \text{H}_2$ and subsequent reactions for HOCOO while RACM2 does not. Sensitivity tests made for realistic atmospheric conditions showed that this reaction was not significant. It could be eliminated to save computational resources.

Acetaldehyde Reactions and Higher Aldehyde Reactions

Acetaldehyde and higher aldehydes photolyze, react with HO radical and react with NO_3 radical. The reaction of aldehydes with nitrate radical is a source of nighttime radicals (Stockwell and Calvert, 1983; Cantrell et al, 1984). The nitrate radical is produced through the reaction of nitrogen dioxide with ozone.



For example, the nitrate radical abstracts a hydrogen atom from formaldehyde to produce nitric acid and CHO radicals. The CHO radical reacts with oxygen to produce hydroperoxy radicals, HO_2 .



For aldehydes with more than one carbon atom acetyl peroxy radicals are produced that may react to produce PAN and its higher homologs.

The three mechanisms treat this chemistry very similarly. The only significant differences are the products produced by higher aldehydes in their photolysis reactions and by their reaction with HO. SAPRC-07 produces several operator radicals while CB05 produces one operator radical and RACM2 produces a surrogate radical species. The SAPRC-07 approach may allow better treatment of some compounds that are aggregated into the RCHO species.

Acetone Reactions and Ketone Reactions

CB05 does not include acetone and other ketones. Given acetone's importance as a radical source at higher altitudes in the troposphere this makes CB05 unsuited for large spatial scale models that need to model the upper troposphere. SAPRC-07 and CB05 differ in their treatment of products. SAPRC-07 produces a large number of operator radicals while RACM2 produces surrogate radical species that participate in the reactions listed for RACM2 in this section. The differing SAPRC-07 and RACM2 methods should lead to similar simulations.

Methanol, Organic Acid and Organic Peroxide Reactions

SAPRC, CB05 and RACM2 include the same reaction for the reaction of methanol with HO. The rate constant in SAPRC-07 and RACM2 are the same while CB05 uses one that is somewhat different.

The treatment of formic acid is the same in all three mechanisms but the treatment of acetic acid is different. SAPRC-07 yields methyl peroxy radical and several operator radicals. CB05 produces only methyl peroxy radical. RACM2 produces methyl peroxy radical and a surrogate radical species for acetic acid. The RACM2 surrogate radical species reactions are listed and they allow RACM2 to more accurately simulate the products of the reaction of acetic acid with HO radical.

The treatment of peroxyacetic and higher peroxycarboxylic acids is very different. For the reaction of HO with peroxyacetic and higher peroxycarboxylic acids CB05 produces only an acetyl peroxy radical while SAPRC-07 additionally produces operator radicals and RACM2 also produces HO, HCHO and an operator radical.

For the reaction of HO with methyl hydrogen peroxide SAPRC-07 and RACM2 were the same, producing HO, HCHO and CH_3O_2 but CB05 incorporates a more highly reactive set of products, HO_2 , CH_3O_2 and an operator peroxy radical. The photolysis reaction of methyl hydrogen peroxide is the same in all three mechanisms. For lumped aggregated organic peroxides with 2 to 4 carbons; the CB05 reactions produce more peroxy radicals than SAPRC-07 and RACM2.

SAPRC-07 includes the reactions of lumped organic peroxides with greater than 5 carbon atoms with HO and its photolysis reactions. Neither CB05 nor RACM2 include a organic peroxide species specifically for organic peroxides with greater than 5 carbon atoms. This may provide some advantage for SAPRC-07 in the modeling of aqueous phase chemistry.

Dicarbonyl Reactions

SAPRC-07 alone includes reactions of biacetyl. CB05 does not include glyoxal. SAPRC-07 and RACM2 include the photolysis and the reactions of glyoxal with HO and nitrate radical. The formulations are different between SAPRC-07 and RACM2 are different. There are three photolysis reactions of glyoxal: a reaction that produces HO_2 and CO; a reaction that produces HCHO and CO; and a third reaction that produces H_2 and CO. RACM2 includes all three but SAPRC-07 omits the third. The RACM2 products of the reactions of glyoxal with HO and nitrate radical include HO_2 , CO and either H_2O or nitric acid. SAPRC-07 forms a higher acyl peroxy radical and a negative quantity of lost carbon. This seems surprising; it is very unclear what purpose this serves. This appears to offset the production of the higher acyl peroxy radical but does subtracting lost carbon add carbon to the system?

Aromatic Products

The three mechanisms treat aromatic chemistry very differently. These reactions show how SAPRC-07 and RACM2 treat aromatic chemistry in much more detail than CB05. The differences in the approaches used in SAPRC-07 and RACM2 are also apparent. The SAPRC-07 AFG-species and the RACM2 DCB-species are used to describe uncharacterized aromatic ring opening products. RACM2 also includes UALD, an unsaturated aldehyde, that has some characteristics of AFG3. In the reactions of all these species SAPRC-07 produces many operator radicals while RACM2 produces surrogate radicals that react through a number of reactions. The RACM2 approach is somewhat easier to understand and more explicit than SAPRC; however both approaches are acceptable within the current state of the science.

Methacrolein, Methyl Vinyl Ketone and Isoprene Products

The products of the reaction of methacrolein with HO, O_3 and NO_3 are very different between the three mechanisms. For example, in the HO reaction RACM2 simply produces an acyl peroxy radical that may react with NO_2 to produce a PAN homologue, react with NO, etc. SAPRC-07 produces half of a peroxy radical from acroleins, MACO3, and a number of operator species. Comparison of the products of the HO-methacrolein reacton in CB05 with SAPRC-07 shows that they are very different. Similar patterns are seen in the products of the O_3 and NO_3 reactions as well. SAPRC-07 and RACM2 treat methyl vinyl ketone while CB05 aggregates it with an isoprene product species. The main difference in the SAPRC-07 and RACM2 treatment of methyl vinyl ketone is the operator approach SAPRC and the semi-explicit approach of RACM2. SAPRC-07 includes reactions for a species that represents lumped isoprene products that is not directly comparable with any in the other two mechanisms.

Reactions of Steady State Operators Used to Represent Radical or Product Formation in Peroxy Radical Reactions

These are unique to SAPRC-07. To support SAPRC-07's operator approach there must be a sufficient number of operators and reactions to represent the production of secondary organic products. This is accomplished in SAPRC-07 by this set of reactions and operators.

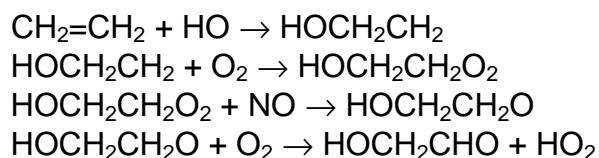
Methane Reaction

All three mechanisms include the reaction of HO with methane. SAPRC-07 and RACM2 use the same rate constant for the reaction while CB05 uses a different expression. There is no significant difference (less than 3.5%) in the temperature range 270 K to 310 K.

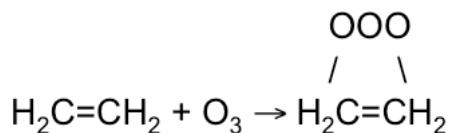
Ethene Reactions

Alkenes are hydrocarbons with at least one double bond. Ethene, $\text{CH}_2=\text{CH}_2$, is the simplest example of an alkene. The reactivity and products of an alkene depends very strongly on the location and number of double bonds. For example, butene may have the double bond located at the end of the molecule, $\text{CH}_2=\text{CHCH}_2\text{CH}_3$ (1-butene), or within the molecule, $\text{CH}_3\text{CH}=\text{CHCH}_3$ (2-butene). In this case the rate parameter for the reaction of hydroxyl radical with 2-butene is greater than its reaction with 1-butene.

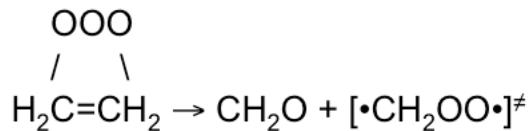
In contrast to alkanes, the hydroxyl radical reacts with alkenes through addition to the double bond. Addition of oxygen occurs to the radical (HOCH_2CH_2) and the resulting peroxy radical ($\text{HOCH}_2\text{CH}_2\text{O}_2$) reacts with nitric oxide to produce nitrogen dioxide and a hydroxy-carbonyl containing compound.



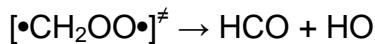
Ozone and nitrate radical also react with alkenes by addition. The reaction of alkenes with ozone produces many products including carbonyl compounds and hydroxyl radical (Horie and Moortgat, 1991; Atkinson and Aschmann, 1993; Atkinson et al, 1995; Seinfeld and Pandis, 1998). These reactions are dominant nighttime sources of hydroxyl radical or where there is little sunlight such as near the bottom of dense forest canopies. For example, the ozone molecule inserts itself across the double bond of ethene.



The product fragments to make formaldehyde and an excited Criegee radical, $[\bullet\text{CH}_2\text{OO}\cdot]^{\ddagger}$.



The excited Criegee radical fragments through several reactions but one leads to the production of hydroxyl radical (Horie and Moortgat, 1991).



Overall the treatment of ethene is within the state-of-the-science in SAPRC-07. SAPRC-07 and RACM2 use the same rate constant for the reaction of ethene with HO radical. The differences in approach between the three mechanisms are clearly visible for ethene. SAPRC-07 produces a several operators that depending upon conditions produce several secondary species. CB05 produces products that are the same and they do not depend upon the concentration of NO_x. RACM2 produces a peroxy radical species that reacts semi-explicitly. SAPRC-07 and RACM2 are more correct than CB05 in the treatment of the reaction of ethene with HO.

For the reaction of ozone with ethene, the products of SAPRC-07 and CB05 are closer than those of RACM2. The production of formaldehyde is accepted but there remains some uncertainty in the decomposition products of the Criegee intermediate. More laboratory research in this area would be helpful. SAPRC-07 and RACM2 use the same rate constants while CB05 uses one that is 10% greater.

The treatment of the reaction of NO₃ with ethene is much more detailed in RACM2 than either SAPRC-07 or CB05. RACM2 produces a NO₃-alkene adduct that represents radicals that react via decomposition and a NO₃-alkene adduct radicals that react to form carbonitrates + HO₂.

SAPRC-07 and CB05 include the reaction of ground state oxygen atom with ethene but RACM2 does not. This may be a remnant of environmental chamber testing; it is probably not significant under most atmospheric conditions.

Isoprene Reactions

The atmospheric oxidation of isoprene is much more complex than ethene with much greater uncertainty associated with the mechanism. Many of the comments pertaining to ethene as implemented in the mechanisms apply to isoprene.

All three mechanisms use the same rate constant for the reaction of isoprene with HO radical. The same differences in approaches as for ethene are there for isoprene. For isoprene SAPRC-07 and SAPRC99 are the same, the mechanisms generate several operators that depending upon conditions produce several secondary species. CB05 produces products that are the same and they do not depend upon the concentration of NO_x. RACM2 produces a peroxy radical species that reacts semi-explicitly. SAPRC-07 and RACM2 are better than CB05 in the treatment of the reaction of isoprene with HO.

The products of the three mechanisms may be less similar for the reaction of ozone with isoprene than for ethene. The yield of HO₂ is much greater in the RACM2 reaction than in SAPRC-07 and CB05. CB05 does not produce methyl vinyl ketene explicitly like the other two. CB05 produces PAR to account for some carbon mass while SAPRC-07 and RACM2 produce organic acids.

SAPRC-07 or CB05 treats the reaction of NO₃ with isoprene similar to their treatment of ethene. RACM2 forms alkylnitrates but neglects the production of any peroxy radical formation. SAPCR-07's treatment is likely to be the most correct.

SAPRC-07 and CB05 include the reaction of ground state oxygen atom with isoprene but RACM2 does not. This may be a remnant of environmental chamber testing; it probably is not significant under most atmospheric conditions.

Acetylene Reactions

SAPRC-07 and RACM2 include the reaction of acetylene with HO radical while CB05 does not. The reaction of acetylene with HO radical and SAPRC-07 and RACM2 are similar. SAPRC-07 also includes the reaction of ozone with acetylene. This is a worthwhile addition to the mechanism given that it adds no extra species to the mechanism.

Benzene Reaction

CB05 does not include benzene as a separate species while SAPRC-07 and RACM2 do. SAPRC-07 and RACM2 use the same rate constant for this reaction. The product yields of many species are different, especially for HO₂. SAPRC-07 uses its operator approach while RACM2 produces a number of products including an organic peroxy radical peculiar to benzene. It is difficult to determine which approach is better given the complex nature of aromatic oxidation.

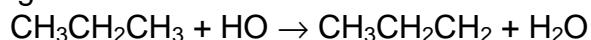
Alkane Reactions

Alkanes are hydrocarbons (contain only hydrogen and carbon atoms) in which the atoms are bonded together with only single bonds. Alkanes include ethane

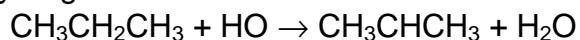
(CH₃CH₃), propane (CH₃CH₂CH₃), n-butane (CH₃CH₂CH₂CH₃) and tertiary-butane (CH₃)₃CH. The hydrogen atoms on the CH₃, CH₂ and CH groups are called primary, secondary and tertiary hydrogen atoms, respectively.

Alkanes react with the hydroxyl radical through abstraction of a hydrogen atom. The hydroxyl radical may abstract any of an alkane's hydrogen atoms but both reactivity differences between the different kinds of hydrogen atoms and the number of the kinds of hydrogen atoms affect the quantity of the different possible products. For alkanes, tertiary hydrogen atoms are more reactive than secondary and secondary hydrogen atoms are more reactive than primary hydrogen atoms. The reactions below illustrate the two possible reaction channels for propane.

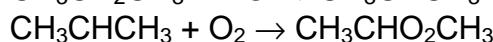
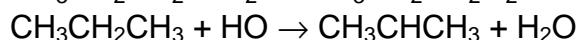
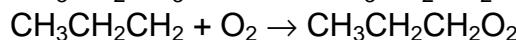
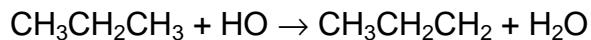
Primary hydrogen abstraction



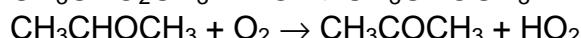
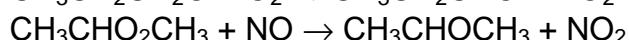
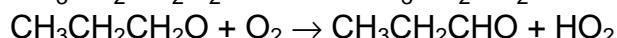
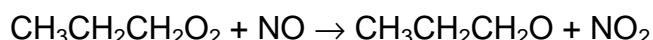
Secondary hydrogen abstraction



The two different radicals react with oxygen to produce two new organic peroxy radicals.



These peroxy radicals react with NO and oxygen to produce acetaldehyde, CH₃CH₂CHO, and acetone, CH₃COCH₃.



CB05 and RACM2 include ethane explicitly. SAPRC-07 includes the species ALK1 that is mostly ethane. For the reaction of HO with ethane SAPRC-07 produced operator radicals; CB05 produces HO₂ and acetaldehyde; and RACM2 makes an ethyl peroxy radical. For higher alkanes SAPRC-07 and RACM2 have similar species but different treatments of their reactions. SAPRC-07 includes ALK2, ALK3, ALK4 and ALK5 while RACM2 includes HC3, HC5 and HC8. CB05 includes a single species, PAR, that represents CH₂ and CH₃ groups in higher alkanes. For the reaction of HO with the higher alkanes the three mechanisms follow schemes that are similar to their schemes for ethane. The treatment used in CB05 is the least realistic.

Alkene Reactions

As discussed for ethene, the differences in approach between the three mechanisms are clearly visible. The rate constants are different but this is expected because there are differences between the three mechanisms in the species aggregated into the alkene species. SAPRC-07 produces several operators that depending upon conditions produce several secondary species. CB05 produces a mix of products that are the same and that do not depend upon the concentration of NO_x. RACM2 produces a peroxy radical species that reacts semi-explicitly. SAPRC-07 and RACM2 are more correct in their approach than CB05 in the treatment of the reaction of alkenes with HO.

For the reaction of ozone with alkenes, the products of the three mechanisms are different. It is difficult to cross compare the reactions used by the mechanisms due to the differences in their aggregation schemes. However, the SAPRC seems acceptable.

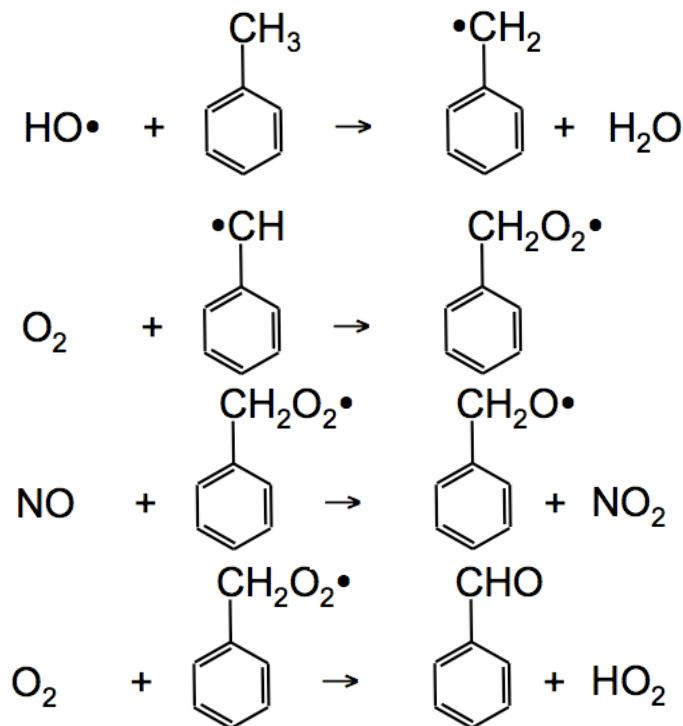
The treatment of the reaction of NO₃ with alkenes in RACM2 produces a NO₃-alkene adduct that represents radicals that react via decomposition and a NO₃-alkene adduct radicals that react to form carbonitrates + HO₂. The RACM2 adjust the yields of these two radicals depending upon the alkene. This seems somewhat better than SAPRC-07 or CB05.

SAPRC-07 and CB05 include the reaction of ground state oxygen atom with alkenes but RACM2 does not. This may be a remnant of environmental chamber testing; it probably is not significant under most atmospheric conditions.

Aromatic Reactions

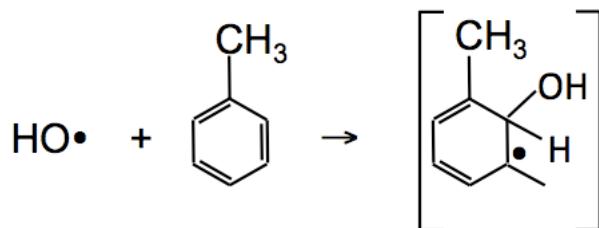
The chemistry of the oxidation of aromatic compounds is too complex to describe in detail in any mechanism that will be routinely used in an air quality model with present day computers. There are at least several hundred reactions for a parent aromatic compound and its reaction products (Calvert et al., 2002). This chemistry remains one of the most heavily parameterized in SAPRC-07, CB05 and RACM2.

The easier aromatic reaction to characterize is the reaction of HO radical with an organic substituent attached to the ring. Near 10% of the hydroxy radicals abstract hydrogen atoms from an alkyl group attached to the ring and the fraction depends upon the number and nature of the substituent groups. If the hydroxy radical reacts with the organic substituent, such as an alkyl group, mechanism follows the chemistry of the substituent group. For example, for toluene if the hydroxyl radical reacts with the methyl group the subsequent chemistry is that of an alkane (Calvert et al., 2002).

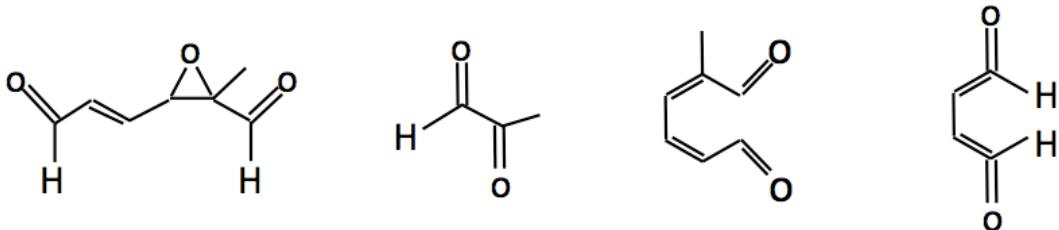


The organic substituents include alkyl, unsaturated-alkene, aldehyde, OH, nitro or other groups. SAPRC-07 adequately treats this chemistry through its operator approach. CB05 uses a highly simplified approach and it is not clear that this aspect of aromatic chemistry is included. RACM2 incorporates a fraction of a peroxy radical species to describe this chemistry.

The most important aromatic reaction with the HO is addition to the ring (Calvert et al., 2002).



The subsequent reactions that follow this reaction break the aromatic ring and produce many organic peroxy radicals, hydroperoxy radicals that convert nitric oxide to nitrogen dioxide and many other highly reactive compounds that contain two carbonyl groups (C=O), (Calvert et al., 2002). Four examples of possible dicarbonyl organic compounds that may result from organic oxidation are shown below.



Terpene Reactions

The treatment of the reactions of terpenes in SAPRC-07, CB05 and RACM2 follow their treatment of other alkenes. SAPRC-07 and CB05 include only one terpene species. RACM2 has a more detailed reaction scheme; RACM2 includes one species for alpha-pinenes and other cyclic terpenes with one double bond and a second species for d-limonene and other cyclic diene-terpenes. Where terpenes are important the RACM2 will be better.

SAPRC-07 Chlorine Reactions

SAPRC-07 is the only one of the mechanisms with chlorine chemistry in the versions that were examined. SAPRC-07 includes the major inorganic reactions of chlorine and the reactions of chlorine atom with organic compounds. The reactions of chlorine are within the state of the science.

Other Remaining Reactions

There were several reactions in CB05 and RACM2 that did not align with SAPRC-07 reactions. These are listed under “Reactions Unique to CB05” and “Reactions Unique to RACM2” in Appendix A.

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Standard Inorganic Reactions

SAPRC07<1> NO2 + hv → NO + O3P # 1.0/SAPRC07<NxO2-06>

CB_05_R1 NO2 + hv → NO + O 1.0 x <NO2_SAPRC99>

RACM2_001 NO2 + hv → O3P + NO

SAPRC07<2> O3P + O2 + M → O3 # 5.68e-34^-2.60

CB_05_R2 O + O2 + M → O3 + M 6.0E-34^-2.4

RACM2_035 O3P + O2 → O3; k = [M]*5.74E-34*(TEMP/300)**(-2.6)

SAPRC07<3> O3P + O3 → # 8.00e-12@2060

CB_05_000 No Equivalent

RACM2_036 O3P + O3 → 2.0 O2; THERMAL A-FACT 8.00E-12 E/R 2060.0

SAPRC07<4> O3P + NO → NO2 # 9.00e-32^-1.50&3.00e-11&0.60&1.0

CB_05_R6 O + NO → NO2 9.0E-32^-1.5 & 3.0E-11

RACM2_046 O3P + NO → NO2; TROE KO 9.00E-32 N 1.5 KINF 3.00E-11 M 0.0

SAPRC07<5> O3P + NO2 → NO # 5.50e-12@-188

CB_05_R4 O + NO2 → NO 5.6E-12 @ -180

RACM2_047 O3P + NO2 → NO + O2; THERMAL A-FACT 5.50E-12 E/R -188.0

SAPRC07<6> O3P + NO2 → NO3 # 2.50e-31^-1.80&2.20e-11^-0.70&0.60&1.0

CB_05_R5 O + NO2 → NO3 2.5E-31^-1.8 & 2.2E-11^-0.7

RACM2_048 O3P + NO2 → NO3; TROE KO 2.50E-31 N 1.8 KINF 2.20E-11 M 0.7

SAPRC07<7> O3 + NO → NO2 # 3.00e-12@1500

CB_05_R3 O3 + NO → NO2 3.0E-12 @ 1500

RACM2_059 O3 + NO → NO2 + O2; THERMAL A-FACT 1.40E-12 E/R 1310.0

SAPRC07<8> O3 + NO2 → NO3 # 1.40e-13@2470

CB_05_R7 NO2 + O3 → NO3 1.2E-13 @ 2450 1

RACM2_060 O3 + NO2 → NO3 + O2; THERMAL A-FACT 1.40E-13 E/R 2470.0

SAPRC07<9> NO + NO3 → 2*NO2 # 1.80e-11@-110

CB_05_R16 NO3 + NO → 2*NO2 1.5E-11 @ -170 1

RACM2_062 NO3 + NO → NO2 + NO2; THERMAL A-FACT 1.80E-11 E/R -110.0

SAPRC07<10> NO + NO + O2 → 2*NO2 # 3.30e-39@-530

CB_05_R22 NO + NO + O2 → 2*NO2 3.3E-39 @ -530

RACM2_061 NO + NO + O2 → NO2 + NO2; THERMAL A-FACT 3.30E-39 E/R -530.0

SAPRC07<11> NO2 + NO3 → N2O5 # 3.60e-30^-4.10&1.90e-12^0.20&0.35&1.0

CB_05_R18 NO3 + NO2 → N2O5 2.0E-30^-4.4 & 1.4E-12^-0.7

RACM2_064 NO3 + NO2 → N2O5; TROE KO 2.00E-30 N 4.4 KINF 1.40E-12 M 0.7

SAPRC07<12> N2O5 → NO2 + NO3 # 1.30e-03^3.50@11000 & 9.70e+14^0.10@11080 & 0.35 & 1.0

CB_05_R21 N2O5 → NO3 + NO2 1E-03^-3.5 @ 11000 & 9.7E14^0.1 @ 11080 & 0.45 & 1.0

RACM2_065 N2O5 → NO2 + NO3; TROE-EQUIL KO 2.20E-30 N 3.9 KINF 1.50E-12 M 0.7 A-FACT 2.70E-27 B 11000.0

SAPRC07<13> N2O5 + H2O → 2*HNO3 # 2.50e-22

CB_05_R19 N2O5 + H2O → 2*HNO3 2.50E-22

RACM2_066 N2O5 + H2O → HNO3 + HNO3; THERMAL A-FACT 2.50E-22 E/R 0.0

SAPRC07<14> N2O5 + H2O + H2O → 2*HNO3 # 1.80e-39

CB_05_R20 N2O5 + H2O+H2O →2*HNO3 1.80E-39

RACM2_000 No Equivalent

SAPRC07<15> NO2 + NO3 → NO + NO2 # 4.50e-14@1260

CB_05_R17 NO3 + NO2 → NO + NO2 4.5E-14 @ 1260

RACM2_063 NO3 + NO2 → NO + NO2 + O2; THERMAL A-FACT 4.50E-14 E/R 1260.0

SAPRC07<16> NO3 + hv → NO # 1.0/SAPRC07<NO3NO-06>

CB_05_R15 NO3 + hv → NO 1.0 x <NO3NO_SAPRC99> 20

RACM2_007 NO3 + hv → NO + O2

SAPRC07<17> NO3 + hv → NO2 + O3P # 1.0/SAPRC07<NO3NO2-6>

CB_05_R14 NO3 + hv → NO2 + O 1.0 x <NO3NO2_SAPRC99>

RACM2_008 NO3 + hv → NO2 + O3P

SAPRC07<18> O3 + hv → O1D # 1.0/SAPRC07<O3O1D-06>

CB_05_R9 O3 + hv → O1D 1.0 x <O3_O1D_IUPAC05>

RACM2_002 O3 + hv → O1D + O2

SAPRC07<19> O3 + hv → O3P # 1.0/SAPRC07<O3O3P-06>

CB_05_R8 O3 + hv → O 1.0 x <O3_O3P_IUPAC05>

RACM2_003 O3 + hv → O3P + O2

SAPRC07<20> O1D + H2O → 2*OH # 1.63e-10

CB_05_R11 O1D + H2O → 2*OH 2.20E-10

RACM2_039 O1D + H2O → HO + HO; THERMAL A-FACT 2.20E-10 E/R 0.0

SAPRC07<21> O1D + M → O3P # 2.38e-11 @ -96

CB_05_R10 O1D + M → O + M 2.1E-11 @ -102

RACM2_037 O1D + N2 → O3P + N2; THERMAL A-FACT 1.80E-11 E/R -107.0

RACM2_038 O1D + O2 → O3P + O2; THERMAL A-FACT 3.20E-11 E/R 0.0

SAPRC07<22> OH + NO → HONO # 7.00e-31^-2.60&3.60e-11^-0.10&0.60&1.0

CB_05_R24 NO + OH → HONO 7.0E-31^-2.6 & 3.6E-11^-0.1

RACM2_049 HO + NO → HONO; TROE KO 7.00E-31 N 2.6 KINF 3.60E-11 M 0.1

SAPRC07<23> HONO + hv → OH + NO # 1.0/SAPRC07<HONO-06>

CB_05_R25 HONO + hv → NO + OH 1.0 x <HONO_IUPAC05>

RACM2_004 HONO + hv → HO + NO

SAPRC07<24> OH + HONO → NO2 # 2.50e-12 @ -260

CB_05_R26 OH + HONO → NO2 1.8E-11 @ 390

RACM2_056 HO + HONO → H2O + NO2; THERMAL A-FACT 2.50E-12 E/R -260.0

SAPRC07<25> OH + NO2 → HNO3 # 1.80e-30^-3.00&2.80e-11&0.60&1.0

CB_05_R28 NO2 + OH → HNO3 2.0E-30^-3.0 & 2.5E-11

RACM2_050 HO + NO2 → HNO3; TROE KO 1.80E-30 N 3.00 KINF 2.80E-11 M 0.0

SAPRC07<26> OH + NO₃ → HO₂ + NO₂ # 2.00e-11

CB_05_R47 NO₃ + OH → HO₂ + NO₂ 2.20E-11

RACM2_051 HO + NO₃ → NO₂ + HO₂; THERMAL A-FACT 2.00E-11 E/R 0.0

SAPRC07<27> OH + HNO₃ → NO₃ %2 # 2.40e-14@-460&2.70e-17@-2199&6.50e-34@-135

CB_05_R29 OH + HNO₃ → NO₃ %2 2.4E-14 @ -460 & 2.7E-17 @ -2199 & 6.5E-34 @ -135

RACM2_057 HO + HNO₃ → NO₃ + H₂O; k₀ = 2.4E-14*EXP(460/TEMP), k₂ = 2.4E-17*EXP(2199/TEMP),
k₃ = 6.5E-34*EXP(1335/TEMP)*[M], k = k₀ + k₃/(1+k₃/k₂)

SAPRC07<28> HNO₃ + hν → OH + NO₂ # 1.0/SAPRC07<HNO₃>

CB_05_R52 HNO₃ + hν → OH + NO₂ 1.0 x <HNO₃_IUPAC05>

RACM2_005 HNO₃ + hν → HO + NO₂

SAPRC07<29> OH + CO → HO₂ + CO₂ %3 # 1.44e-13@0&3.43e-33@0

CB_05_R65 OH + CO → HO₂ %3 1.44E-13 @ 0.0 & 3.43E-33 @ 0.0

RACM2_070 CO + HO → HO₂ + CO₂; k = 1.44E-13*(1.+0.8*[M]/4E19)

SAPRC07<30> OH + O₃ → HO₂ # 1.70e-12@940

CB_05_R12 O₃ + OH → HO₂ 1.7E-12 @ 940

RACM2_040 O₃ + HO → HO₂ + O₂; THERMAL A-FACT 1.70E-12 E/R 940.0

SAPRC07<31> HO₂ + NO → OH + NO₂ # 3.60e-12@-270

CB_05_R30 HO₂ + NO → OH + NO₂ 3.5E-12 @ -250

RACM2_052 HO₂ + NO → NO₂ + HO; THERMAL A-FACT 3.60E-12 E/R -270.0

SAPRC07<32> HO₂ + NO₂ → HNO₄ # 2.00e-31^-3.40&2.90e-12^-1.10&0.60&1.0

CB_05_R31 HO₂ + NO₂ → PNA 1.8E-31^-3.2 & 4.7E-12 & 0.6

RACM2_053 HO₂ + NO₂ → HNO₄; TROE KO 2.0E-31 N 3.4 KINF 2.90E-12 M 1.1

SAPRC07<33> HNO₄ → HO₂ + NO₂ # 3.72e-05^-2.40@10650&5.42e+15^-2.30@11170&0.60&1.0

CB_05_R32 PNA → HO₂ + NO₂ 4.1E-5 @ 10650 & 4.8E15 @ 11170 & 0.6

RACM2_054 HNO₄ → HO₂ + NO₂; TROE-EQUIL KO 2.00E-31 N 3.4 KINF 2.90E-12 M 1.1 A-FACT 2.10E-27 B 10900.

SAPRC07<34> HNO4 + hv → 0.61*HO2 + 0.61*NO2 + 0.39*OH + 0.39*NO3 # 1.0/SAPRC07<HNO4-06>
CB_05_R51 PNA + hv → 0.610*HO2 + 0.610*NO2 + 0.390*OH + 0.390*NO3 1.0 x <HO2NO2_IUPAC05>
RACM2_006 HNO4 + hv → 0.80 HO2 + 0.80 NO2 + 0.20 HO + 0.20 NO3

SAPRC07<35> HNO4 + OH → NO2 # 1.30e-12@-380
CB_05_R33 OH + PNA → NO2 1.3E-12 @ -380
RACM2_058 HO + HNO4 → NO2 + H2O + O2; THERMAL A-FACT 1.30E-12 E/R -380.0

SAPRC07<36> HO2 + O3 → OH # 2.03e-16^4.57@-636
CB_05_R13 O3 + HO2 → OH 1.0E-14 @ 490
RACM2_041 O3 + HO2 → HO + 2. O2; THERMAL A-FACT 1.00E-14 E/R 490.0

SAPRC07<37> HO2 + HO2 → HO2H %3 # 2.20e-13@-600&1.90e-33@-980
CB_05_R34 HO2 + HO2 → H2O2 %3 2.3E-13 @ -600 & 1.7E-33 @ -1000
RACM2_044 HO2 + HO2 → H2O2 + O2; k = 2.2E-13*EXP(600./TEMP) +1.90E-33*[M]*EXP(980./TEMP)

SAPRC07<38> HO2 + HO2 + H2O → HO2H %3 # 3.08e-34@-2800&2.66e-54@-3180
CB_05_R35 HO2 + HO2 + H2O → H2O2 %3 3.22E-34 @ -2800 & 2.38E-54 @ -3200
RACM2_045 HO2 + HO2 + H2O → H2O2 + H2O + O2; k = 3.08E-34*EXP(2800./TEMP)+2.59E-54*[M]*EXP(3180./TEMP)

SAPRC07<39> NO3 + HO2 → 0.8*OH + 0.8*NO2 + 0.2*HNO3 # 4.00e-12
CB_05_R48 NO3 + HO2 → HNO3 3.50E-12
RACM2_055 HO2 + NO3 → 0.3 HNO3 + 0.7 NO2 + 0.7 HO; THERMAL A-FACT 4.00E-12 E/R 0.0

SAPRC07<40> NO3 + NO3 → 2*NO2 # 8.50e-13@2450
CB_05_R50 NO3 + NO3 → 2*NO2 8.5E-13 @ 2450
RACM2_067 NO3 + NO3 → NO2 + NO2 + O2; THERMAL A-FACT 8.50E-13 E/R 2450.0

SAPRC07<41> HO2H + hv → 2*OH # 1.0/SAPRC07<H2O2>
CB_05_R36 H2O2 + hv → 2*OH 1.0 x <H2O2_SAPRC99>
RACM2_009 H2O2 + hv → HO + HO

SAPRC07<42> HO₂H + OH → HO₂ # 1.80e-12

CB_05_R37 OH + H₂O₂ → HO₂ 2.9E-12 @ 160

RACM2_043 H₂O₂ + HO → HO₂ + H₂O; THERMAL A-FACT 2.90E-12 E/R 160.0

SAPRC07<43> OH + HO₂ → # 4.80e-11@-250

CB_05_R43 OH + HO₂ → 4.8E-11 @ -250

RACM2_042 HO + HO₂ → H₂O + O₂; THERMAL A-FACT 4.80E-11 E/R -250.0

SAPRC07<44> OH + SO₂ → HO₂ + SULF # 3.30e-31^-4.30&1.60e-12&0.60&1.0

CB_05_R153 SO₂ + OH → SULF + HO₂ 3.0E-31^-3.3 & 1.5E-12

RACM2_069 HO + SO₂ → SULF + HO₂; TROE KO 3.30E-31 N 4.3 KINF 1.60E-12 M 0.0

SAPRC07<45> OH + H₂ → HO₂ # 7.70e-12@2100

CB_05_R39 OH + H₂ → HO₂ 5.5E-12 @ 2000

RACM2_068 HO + H₂ → H₂O + HO₂; THERMAL A-FACT 7.70E-12 E/R 2100.0

Methyl Peroxy Radical Reactions

SAPRC07<BR01> MEO₂ + NO → NO₂ + HCHO + HO₂ # 2.30e-12@-360

CB_05_R67 MEO₂ + NO → FORM + HO₂ + NO₂ 2.8E-12 @ -300

RACM2_191 MO₂ + NO → HCHO + HO₂ + NO₂; THERMAL A-FACT 2.80E-12 E/R -300.0

SAPRC07<BR02> MEO₂ + HO₂ → COOH # 3.46e-13^0.36@-780

CB_05_R68 MEO₂ + HO₂ → MEPX 4.1E-13 @ -750

RACM2_215 MO₂ + HO₂ → OP1; THERMAL A-FACT 4.10E-13 E/R -750.0

SAPRC07<BR03> MEO₂ + HO₂ → HCHO # 3.34e-14^-3.53@-780

CB_05_000 No Equivalent

RACM2_000 No Equivalent

SAPRC07<BR04> MEO₂ + NO₃ → HCHO + HO₂ + NO₂ # 1.30e-12

CB_05_000 No Equivalent

RACM2_306 MO₂ + NO₃ → HCHO + HO₂ + NO₂; THERMAL A-FACT 1.20E-12 E/R 0.0

SAPRC07<BR05> MEO2 + MEO2 → MEOH + HCHO # 6.39e-14^-1.80@-365

SAPRC07<BR06> MEO2 + MEO2 → 2*HCHO + 2*HO2 # 7.40e-13@520

CB_05_R69 MEO2 + MEO2 → 1.370*FORM + 0.740*HO2 + 0.630*MEOH 9.5E-14 @ -390

RACM2_240 MO2 + MO2 → 1.37 HCHO + 0.74 HO2 + 0.63 MOH; THERMAL A-FACT 9.50E-14 E/R -390.0

RO2C and Other Active Peroxy Radical Operators

SAPRC07<BR07> RO2C + NO → NO2 # 2.60e-12@-380

CB_05_R54 XO2 + NO → NO2 2.6E-12 @ -365

CB_05_R129 TO2 + NO → 0.900*NO2 + 0.900*HO2 + 0.900*OPEN + 0.100*NTR 8.10E-12

RACM2_342 XO2 + NO → NO2; THERMAL A-FACT 4.00E-12 E/R 0.0

SAPRC07<BR08> RO2C + HO2 → # 3.80e-13@-900

CB_05_R56 XO2 + HO2 → ROOH 7.5E-13 @ -700

RACM2_338 XO2 + HO2 → OP2; THERMAL A-FACT 1.66E-13 E/R -1300.0

SAPRC07<BR09> RO2C + NO3 → NO2 # 2.30e-12

CB_05_000 No Equivalent

RACM2_343 XO2 + NO3 → NO2; THERMAL A-FACT 1.20E-12 E/R 0.0

SAPRC07<BR10> RO2C + MEO2 → 0.5*RO2C + 0.5*xHO2 + 0.5*xHCHO + 0.25*HCHO + 0.25*MEOH # 2.00e-13

CB_05_000 No Equivalent

RACM2_339 XO2 + MO2 → HCHO + HO2; THERMAL A-FACT 5.99E-15 E/R -1510.0

SAPRC07<BR11> RO2C + RO2C → # 3.50e-14

CB_05_R58 XO2 + XO2 → 6.80E-14

RACM2_341 XO2 + XO2 → THERMAL A-FACT 7.13E-17 E/R -2950.0

SAPRC07<BR12> RO2XC + NO → XN # 1.0*KSAPRC07<BR07>

CB_05_000 No Equivalent

RACM2_000 No Equivalent

SAPRC07<BR13> RO2XC + HO2 → # 1.0*KSAPRC07<BR08>

CB_05_000 No Equivalent

RACM2_000 No Equivalent

SAPRC07<BR14> RO2XC + NO3 → NO2 # 1.0*Ksaprc07<BR09>

CB_05_000 No Equivalent

RACM2_000 No Equivalent

SAPRC07<BR15> RO2XC + MEO2 → 0.5*RO2C + 0.5*xHO2 + 0.5*xHCHO + 0.25*HCHO + 0.25*MEOH #
1.0*Ksaprc07<BR10>

CB_05_000 No Equivalent

RACM2_000 No Equivalent

SAPRC07<BR16> RO2XC + RO2C → # 1.0*Ksaprc07<BR11>

CB_05_000 No Equivalent

RACM2_000 No Equivalent

SAPRC07<BR17> RO2XC + RO2C → # 1.0*Ksaprc07<BR11>

CB_05_000 No Equivalent

RACM2_000 No Equivalent

Reactions Involving PAN, Homologues and Acyl Peroxy Radicals

SAPRC07<BR18> MECO3 + NO2 → PAN # 2.70e-28^-7.10&1.21e-11^-0.90&0.30&1.0

CB_05_R88 C2O3 + NO2 → PAN 2.7E-28^-7.1 & 1.2E-11^-0.9 & 0.3

RACM2_185 ACO3 + NO2 → PAN; TROE KO 8.50E-29 N 6.5 KINF 1.10E-11 M 1.0

SAPRC07<BR19> PAN → MECO3 + NO2 # 4.90e-03@12100&4.00e+16@13600&0.30&1.0

CB_05_R89 PAN → C2O3 + NO2 4.9E-3 @ 12100 & 5.4E16 @ 13830 & 0.3

RACM2_187 PAN → ACO3 + NO2; TROE-EQUIL KO 9.70E-29 N 5.6 KINF 9.30E-12 M 1.5; THERMAL A-FACT 8.60E-29 B 13954.

SAPRC07<BR20> PAN + hv → 0.6*MECO3 + 0.6*NO2 + 0.4*MEO2 + 0.4*CO2 + 0.4*NO3 # 1.0/SAPRC07<PAN>

CB_05_R90 PAN + hv → C2O3 + NO2 1.0 x <PAN_IUPAC05>

RACM2_033 PAN + hv → ACO3 + NO2

RACM2_034 PAN + hv → MO2 + CO2 + NO3

SAPRC07<BR21> MECO3 + NO → MEO2 + CO2 + NO2 # 7.50e-12@-290
CB_05_R87 C2O3 + NO → MEO2 + NO2 8.1E-12 @ -270
RACM2_209 ACO3 + NO → MO2 + NO2; THERMAL A-FACT 8.10E-12 E/R -270

SAPRC07<BR22> MECO3 + HO2 → AACD + 0.3*O3 # 5.20e-13@-980
CB_05_R91 C2O3 + HO2 → 0.800*PACD + 0.200*AACD + 0.200*O3 4.3E-13 @ -1040
RACM2_233 ACO3 + HO2 → 0.4 PAA + 0.2 ORA2 + 0.4 MO2 + 0.4 HO + 0.4 CO2; THERMAL A-FACT 4.3E-13 E/R -1040.

SAPRC07<BR23> MECO3 + NO3 → MEO2 + CO2 + NO2 # 1.0*KSAPRC07<BR09>
CB_05_000 No Equivalent
RACM2_320 ACO3 + NO3 → MO2 + NO2; THERMAL A-FACT 4.00E-12 E/R 0.0

SAPRC07<BR24> MECO3 + MEO2 → 0.9*AACD + 0.9*HCHO + 0.1*HCHO + 0.1*HO2 + 0.1*MEO2 +
0.1*CO2 # 2.00e-12@-500
CB_05_R92 C2O3 + MEO2 → 0.900*MEO2 + 0.900*HO2 + FORM + 0.100*AACD 2.0E-12 @ -500
RACM2_265 ACO3 + MO2 → HCHO + 0.9 HO2 + 0.90 MO2 + 0.1 ORA2 + 0.4 CO2; THERMAL A-FACT 2.0E-11 E/R -500.0

SAPRC07<BR25> MECO3 + RO2C → AACD # 4.40e-13@-1070
CB_05_R93 C2O3 + XO2 → 0.900*MEO2 + 0.100*AACD 4.4E-13 @ -1070
RACM2_340 XO2 + ACO3 → MO2; THERMAL A-FACT 3.40E-14 E/R -1560.0

SAPRC07<BR26> MECO3 + RO2XC → AACD # 1.0*KSAPRC07<BR25>
CB_05_000 No Equivalent
RACM2_000 No Equivalent

SAPRC07<BR27> MECO3 + MECO3 → 2*MEO2 + 2*CO2 # 2.90e-12@-500
CB_05_R94 C2O3 + C2O3 → 2*MEO2 2.9E-12 @ -500
RACM2_296 ACO3 + ACO3 → 2.0 MO2 + 2.0 CO2; THERMAL A-FACT 2.50E-12 E/R -500.0

SAPRC07<BR28> RCO3 + NO2 → PAN2 # 1.21e-11^-1.07@0
CB_05_R103 CXO3 + NO2 → PANX 2.7E-28^-7.1 & 1.2E-11^-0.9 & 0.3
RACM2_186 RCO3 + NO2 → PPN; TROE KO 8.50E-29 N 6.5 KINF 1.10E-11 M 1.0

SAPRC07<BR29> PAN2 → RCO3 + NO2 # 8.30e+16@13940

CB_05_R104 PANX → CXO3 + NO2 4.9E-3 @ 12100 & 5.4E16 @ 13830 & 0.3

RACM2_188 PPN → RCO3 + NO2

TROE-EQUIL KO 9.70E-29 N 5.6 KINF 9.30E-12 M 1.5; THERMAL A-FACT 8.60E-29 B 13954.

SAPRC07<BR30> PAN2 + hv → 0.6*RCO3 + 0.6*NO2 + 0.4*RO2C + 0.4*xHO2 + 0.4*yROOH + 0.4*xCCHO + 0.4*CO2 + 0.4*NO3 # 1.0/SAPRC07<PAN>

CB_05_R105 PANX + hv → CXO3 + NO2 1.0 x <PAN_IUPAC05>

RACM2_000 No Equivalent

SAPRC07<BR31> RCO3 + NO → NO2 + RO2C + xHO2 + yROOH + xCCHO + CO2 # 6.70e-12@-340

CB_05_R102 CXO3 + NO → ALD2 + NO2 + HO2 + XO2 6.7E-12 @ -340

RACM2_210 RCO3 + NO → ETPH + NO2; THERMAL A-FACT 8.10E-12 E/R -270

SAPRC07<BR32> RCO3 + HO2 → PACD + 0.25*O3 # 1.0*KSAPRC07<BR22>

CB_05_R107 CXO3 + HO2 → 0.800*PACD + 0.200*AACD + 0.200*O3 4.3E-13 @ -1040

RACM2_234 RCO3 + HO2 → 0.4 PAA + 0.2 ORA2 + 0.4 ETPH + 0.4 HO + 0.4 CO2; THERMAL A-FACT 4.3E-13 E/R -1040

SAPRC07<BR33> RCO3 + NO3 → NO2 + RO2C + xHO2 + yROOH + xCCHO + CO2 # 1.0*KSAPRC07<BR09>

CB_05_000 No Equivalent

RACM2_321 RCO3 + NO3 → ETPH + NO2; THERMAL A-FACT 4.00E-12 E/R 0.0

SAPRC07<BR34> RCO3 + MEO2 → PACD + HCHO # 1.0*KSAPRC07<BR24>

CB_05_R108 CXO3 + MEO2 → 0.900*ALD2 + 0.900*XO2 + HO2 + 0.100*AACD + 0.100*FORM 2.0E-12 @ -500

RACM2_266 RCO3 + MO2 → HCHO + 0.9 HO2 + 0.9 MO2 + 0.1 ORA2 + 0.4 CO2; THERMAL A-FACT 2.0E-11 E/R -500.0

SAPRC07<BR35> RCO3 + RO2C → PACD # 1.0*KSAPRC07<BR25>

CB_05_R109 CXO3 + XO2 → 0.900*ALD2 + 0.100*AACD 4.4E-13 @ -1070

RACM2_000 No Equivalent

SAPRC07<BR36> RCO3 + RO2XC → PACD # 1.0*KSAPRC07<BR25>

CB_05_000 No Equivalent

RACM2_000 No Equivalent

SAPRC07<BR37> RCO3 + MECO3 → 2*CO2 + MEO2 + RO2C + xHO2 + yROOH + xCCHO # 1.0*KSAPRC07<BR27>
CB_05_R111 CXO3 + C2O3 → MEO2 + XO2 + HO2 + ALD2 2.9E-12 @ -500
RACM2_000 No Equivalent

SAPRC07<BR38> RCO3 + RCO3 → 2*RO2C + 2*xHO2 + 2*xCCHO + 2*yROOH + 2*CO2 # 1.0*KSAPRC07<BR27>
CB_05_R110 CXO3 + CXO3 → 2*ALD2 + 2*XO2 + 2*HO2 2.9E-12 @ -500
RACM2_297 RCO3 + RCO3 → 2.0 ETPH + 2.0 CO2; THERMAL A-FACT 2.50E-12 E/R -500.0

SAPRC07<BR39> BZCO3 + NO2 → PBZN # 1.37e-11
CB_05_000 No Equivalent
RACM2_000 No Equivalent

SAPRC07<BR40> PBZN → BZCO3 + NO2 # 7.90e+16@14000
CB_05_000 No Equivalent
RACM2_000 No Equivalent

SAPRC07<BR41> PBZN → 0.6*BZCO3 + 0.6*NO2 + 0.4*CO2 + 0.4*BZO + 0.4*RO2C + 0.4*NO3
1.0/SAPRC07<PAN>
CB_05_000 No Equivalent
RACM2_000 No Equivalent

SAPRC07<BR42> BZCO3 + NO → NO2 + CO2 + BZO + RO2C # 1.0*KSAPRC07<BR31>
CB_05_000 No Equivalent
RACM2_110 BALP + NO → BAL1 + NO2; THERMAL A-FACT 4.00E-12 E/R 0.0

SAPRC07<BR43> BZCO3 + HO2 → PACD + 0.25*O3 + 4*XC # 1.0*KSAPRC07<BR22>
CB_05_000 No Equivalent
RACM2_000 No Equivalent

SAPRC07<BR44> BZCO3 + NO3 → NO2 + CO2 + BZO + RO2C # 1.0*KSAPRC07<BR09>
CB_05_000 No Equivalent
RACM2_335 BALP + NO3 → BAL1 + NO2; THERMAL A-FACT 1.20E-12 E/R 0.0
RACM2_336 BAL1 + NO3 → BAL2 + NO2; THERMAL A-FACT 1.20E-12 E/R 0.0

SAPRC07<BR45> BZCO3 + MEO2 → PACD + HCHO + 4*XC # 1.0*KSAPRC07<BR24>

CB_05_000 No Equivalent

RACM2_262 BALP + MO2 → HCHO + HO2 + BAL1; THERMAL A-FACT 3.56E-14 E/R -708.

RACM2_263 BAL1 + MO2 → HCHO + HO2 + BAL2; THERMAL A-FACT 3.56E-14 E/R -708.

SAPRC07<BR46> BZCO3 + RO2C → PACD + 4*XC # 1.0*KSAPRC07<BR25>

CB_05_000 No Equivalent

RACM2_000 No Equivalent

SAPRC07<BR47> BZCO3 + RO2XC → PACD + 4*XC # 1.0*KSAPRC07<BR25>

CB_05_000 No Equivalent

RACM2_290 BALP + ACO3 → BAL1 + MO2; THERMAL A-FACT 7.40E-13 E/R -765.

RACM2_291 BAL1 + ACO3 → BAL2 + MO2; THERMAL A-FACT 7.40E-13 E/R -765.

SAPRC07<BR48> BZCO3 + MECO3 → 2*CO2 + MEO2 + BZO + RO2C # 1.0*KSAPRC07<BR27>

CB_05_000 No Equivalent

RACM2_000 No Equivalent

**SAPRC07<BR49> BZCO3 + RCO3 → 2*CO2 + RO2C + xHO2 + yROOH + xCCHO + BZO + RO2C
1.0*KSAPRC07<BR27>**

CB_05_000 No Equivalent

RACM2_000 No Equivalent

SAPRC07<BR50> BZCO3 + BZCO3 → 2*BZO + 2*RO2C + 2*CO2 # 1.0*KSAPRC07<BR27>

CB_05_000 No Equivalent

RACM2_000 No Equivalent

PAN Homologue from Methacrolein and Peroxy Radicals from Acroleins

SAPRC07<BR51> MACO3 + NO2 → MAPAN # 1.0*KSAPRC07<BR28>

CB_05_000 No Equivalent

RACM2_189 MACP + NO2 → MPAN; THERMAL A-FACT 2.80E-12 E/R -181.

SAPRC07<BR52> MAPAN → MACO3 + NO2 # 1.60e+16@13486

CB_05_000 No Equivalent

RACM2_190 MPAN → MACP + NO2; THERMAL A-FACT 1.60E+16 E/R 13486.

SAPRC07<BR53> MAPAN + hv → 0.6*MACO3 + 0.6*NO2 + 0.4*CO2 + 0.4*HCHO + 0.4*MEO3 + 0.4*NO3
1.0/SAPRC07<PAN>

CB_05_000 No Equivalent

RACM2_000 No Equivalent

SAPRC07<BR54> MACO3 + NO → NO2 + CO2 + HCHO + MECO3 # 1.0*KSAPRC07<BR31>

CB_05_000 No Equivalent

RACM2_200 MACP + NO → NO2 + 0.25 ACO3 + 0.25 HACE + 0.25 CO + 0.75 HCHO + 0.50 MGLY + 0.75 HO2;
THERMAL A-FACT 2.54E-12 E/R -360.

SAPRC07<BR55> MACO3 + HO2 → PACD + 0.25*O3 + XC # 1.0*KSAPRC07<BR22>

CB_05_000 No Equivalent

RACM2_224 MACP + HO2 → MAHP; THERMAL A-FACT 1.82E-13 E/R -1300.

SAPRC07<BR56> MACO3 + NO3 → NO2 + CO2 + HCHO + MECO3 # 1.0*KSAPRC07<BR09>

CB_05_000 No Equivalent

RACM2_328 MACP + NO3 → NO2 + 0.33 ACO3 + 0.33 HACE + 0.33 CO + HCHO + 0.667 MGLY + HO2; THERMAL A-
FACT 1.20E-12 E/R 0.0

SAPRC07<BR57> MACO3 + MEO2 → PACD + HCHO + XC # 1.0*KSAPRC07<BR24>

CB_05_000 No Equivalent

RACM2_249 MACP + MO2 → 1.50 HCHO + HO2 + 0.167 HACE + 0.167 CO + 0.167 ACO3 + 0.333 MGLY + 0.042
ORA2 + 0.250 MOH + 0.250 ROH; THERMAL A-FACT 3.40E-14 E/R -221.

SAPRC07<BR58> MACO3 + RO2C → PACD + XC # 1.0*KSAPRC07<BR25>

CB_05_000 No Equivalent

RACM2_000 No Equivalent

SAPRC07<BR59> MACO3 + RO2XC → PACD + XC # 1.0*KSAPRC07<BR25>

CB_05_000 No Equivalent

RACM2_000 No Equivalent

SAPRC07<BR60> MACO3 + MECO3 → 2*CO2 + MEO2 + HCHO + MECO3 # 1.0*KSAPRC07<BR27>

CB_05_000 No Equivalent

RACM2_280 MACP + ACO3 → 0.500 HO2 + 0.5 MO2 + 0.583 ORA2 + 0.167 HACE + 0.167 CO + 0.167 ACO3 + 0.33 MGLY + HCHO; THERMAL A-FACT 8.40E-14 E/R -221.

**SAPRC07<BR61> MACO3 + RCO3 → HCHO + MECO3 + RO2C + xHO2 + yROOH + xCCHO + 2*CO2
1.0*KSAPRC07<BR27>**

CB_05_000 No Equivalent

RACM2_000 No Equivalent

SAPRC07<BR62> MACO3 + BZCO3 → HCHO + MECO3 + BZO + RO2C + 2*CO2 # 1.0*KSAPRC07<BR27>

CB_05_000 No Equivalent

RACM2_000 No Equivalent

SAPRC07<BR63> MACO3 + MACO3 → 2*HCHO + 2*MEO3 + 2*CO2 # 1.0*KSAPRC07<BR27>

CB_05_000 No Equivalent

RACM2_000 No Equivalent

t-Butoxy Radical Reactions

SAPRC07<BR64> TBUO + NO2 → RNO3 + -2*XC # 2.40e-11

CB_05_000 No Equivalent

RACM2_000 No Equivalent

SAPRC07<BR65> TBUO → ACET + MEO2 # 7.50e+14@8152

CB_05_000 No Equivalent

RACM2_000 No Equivalent

Phenoxy Radicals

SAPRC07<BR66> BZO + NO2 → NPHE # 2.30e-11@-150

CB_05_R133 CRO + NO2 → NTR 1.40E-11

RACM2_184 CHO + NO2 → ONIT; THERMAL A-FACT 2.00E-11 E/R 0.0

SAPRC07<BR67> BZO + HO2 → CRES + -1*XC # 1.0*Ksaprc07<BR08>

CB_05_R134 CRO + HO2 → CRES 5.50E-12

RACM2_232 CHO + HO2 → CSL; THERMAL A-FACT 1.00E-11 E/R 0.0

SAPRC07<BR68> BZO → CRES + RO2C + xHO2 + -1*XC # 1.00e-03

CB_05_R130 TO2 → CRES + HO2 4.2

RACM2_000 No Equivalent

Steady State Operators for Representing Radical or Product Formation in Peroxy Radical Reactions

SAPRC07<RO01> xHO2 → HO2 # 'RO2RO'

CB_05_000 No Equivalent

RACM2_000 No Equivalent

SAPRC07<RO02> xHO2 → # 'RO2XRO'

CB_05_000 No Equivalent

RACM2_000 No Equivalent

SAPRC07<RO03> xOH → OH # 'RO2RO'

CB_05_000 No Equivalent

RACM2_000 No Equivalent

SAPRC07<RO04> xOH → # 'RO2XRO'

CB_05_000 No Equivalent

RACM2_000 No Equivalent

SAPRC07<RO05> xNO2 → NO2 # 'RO2RO'

CB_05_000 No Equivalent

RACM2_000 No Equivalent

SAPRC07<RO06> xNO2 → XN # 'RO2XRO'

CB_05_000 No Equivalent

RACM2_000 No Equivalent

SAPRC07<RO07> xMEO2 → MEO2 # 'RO2RO'

CB_05_000 No Equivalent

RACM2_000 No Equivalent

SAPRC07<RO08> xMEO2 → XC # 'RO2XRO'

CB_05_000 No Equivalent

RACM2_000 No Equivalent

SAPRC07<RO09> xMECO3 → MECO3 # 'RO2RO'

CB_05_000 No Equivalent

RACM2_000 No Equivalent

SAPRC07<RO10> xMECO3 → 2*XC # 'RO2XRO'

CB_05_000 No Equivalent

RACM2_000 No Equivalent

SAPRC07<RO11> xRCO3 → RCO3 # 'RO2RO'

CB_05_000 No Equivalent

RACM2_000 No Equivalent

SAPRC07<RO12> xRCO3 → 3*XC # 'RO2XRO'

CB_05_000 No Equivalent

RACM2_000 No Equivalent

SAPRC07<RO13> xMACO3 → MACO3 # 'RO2RO'

CB_05_000 No Equivalent

RACM2_000 No Equivalent

SAPRC07<RO14> xMACO3 → 4*XC # 'RO2XRO'

CB_05_000 No Equivalent

RACM2_000 No Equivalent

SAPRC07<RO15> xTBUO → TBUO # 'RO2RO'

CB_05_000 No Equivalent

RACM2_000 No Equivalent

SAPRC07<RO16> xTBUO → 4*XC # 'RO2XRO'

CB_05_000 No Equivalent

RACM2_000 No Equivalent

SAPRC07<RO17> xCO → CO # 'RO2RO'

CB_05_000 No Equivalent

RACM2_000 No Equivalent

SAPRC07<RO18> xCO → XC # 'RO2XRO'

CB_05_000 No Equivalent

RACM2_000 No Equivalent

Formaldehyde Reactions

SAPRC07<BP01> HCHO + hν → 2*HO2 + CO # 1.0/SAPRC07<HCHOR-06>

CB_05_R74 FORM + hν → 2*HO2 + CO 1.0 x <HCHO_R_SAPRC99>

RACM2_011 HCHO + hν → HO2 + HO2 + CO

SAPRC07<BP02> HCHO + hν → CO # 1.0/SAPRC07<HCHOM-06>

CB_05_R75 FORM + hν → CO 1.0 x <HCHO_M_SAPRC99>

RACM2_010 HCHO + hν → H2 + CO

SAPRC07<BP03> HCHO + OH → HO2 + CO # 5.40e-12@-135

CB_05_R73 FORM + OH → HO2 + CO 9.00E-12

RACM2_124 HCHO + HO → HO2 + CO + H2O; THERMAL A-FACT 5.50E-12 E/R -125.0

SAPRC07<BP04> HCHO + HO2 → HOCOO # 9.70e-15@-625

CB_05_R78 FORM + HO2 → HCO3 9.7E-15 @ -625 2

RACM2_000 No Equivalent

SAPRC07<BP05> HOCOO → HO2 + HCHO # 2.40e+12@7000

CB_05_R79 HCO3 → FORM + HO2 2.4E+12 @ 7000

RACM2_000 No Equivalent

SAPRC07<BP06> HOCOO + NO → FACD + NO₂ + HO₂ # 1.0*KSAPRC07<BR01>

CB_05_R80 HCO₃ + NO → FACD + NO₂ + HO₂ 5.60E-12

RACM2_000 No Equivalent

SAPRC07<BP07> HCHO + NO₃ → HNO₃ + HO₂ + CO # 2.00e-12@2431

CB_05_R77 FORM + NO₃ → HNO₃ + HO₂ + CO 5.80E-16

RACM2_149 HCHO + NO₃ → HO₂ + HNO₃ + CO; THERMAL A-FACT 2.00E-12 E/R 2440.0

Acetaldehyde Reactions and Higher Aldehyde Reactions

SAPRC07<BP08> CCHO + OH → MECO₃ # 4.40e-12@-365

CB_05_R84 ALD2+OH → C₂O₃ 5.6E-12 @ -270

RACM2_125 ACD + HO → ACO₃ + H₂O; THERMAL A-FACT 4.38E-12 E/R -366.0

SAPRC07<BP09> CCHO + hν → CO + HO₂ + MEO₂ # 1.0/SAPRC07<CCHO_R>

CB_05_R86 ALD2 + hν → MEO₂ + CO + HO₂ 1.0 x <CCHO_R_SAPRC99> 20

RACM2_012 ACD + hν → MO₂ + HO₂ + CO

SAPRC07<BP10> CCHO + NO₃ → HNO₃ + MECO₃ # 1.40e-12@1860

CB_05_R85 ALD2 + NO₃ → C₂O₃ + HNO₃ 1.4E-12 @ 1900

RACM2_150 ACD + NO₃ → ACO₃ + HNO₃; THERMAL A-FACT 1.40E-12 E/R 1900.0

SAPRC07<BP11> RCHO + OH → 0.965*RCO₃ + 0.035*RO₂C + 0.035*xHO₂ + 0.035*xCO + 0.035*xCCHO + 0.035*yROOH # 5.10e-12@-405

CB_05_R99 ALDX + OH → CXO₃ 5.1E-12 @ -405

RACM2_126 ALD + HO → RCO₃ + H₂O; THERMAL A-FACT 5.10E-12 E/R -405.0

SAPRC07<BP12> RCHO + hν → RO₂C + xHO₂ + yROOH + xCCHO + CO + HO₂ # 1.0/SAPRC07<C₂CHO>

CB_05_R101 ALDX + hν → MEO₂ + CO + HO₂ 1.0 x <C₂CHO_SAPRC99>

RACM2_013 ALD + hν → ETP + HO₂ + CO

SAPRC07<BP13> RCHO + NO₃ → HNO₃ + RCO₃ # 1.40e-12@1601

CB_05_R100 ALDX + NO₃ → CXO₃ + HNO₃ 6.50E-15

RACM2_151 ALD + NO₃ → RCO₃ + HNO₃; THERMAL A-FACT 3.76E-12 E/R 1900.0

Acetone Reactions and Ketone Reactions

SAPRC07<BP14> ACET + OH → RO2C + xMECO3 + xHCHO + yROOH # 4.56e-14^3.65@-429

CB_05_000 No Equivalent

RACM2_127 ACT + HO → ACTP + H2O; k = 1.39E-13+3.72E-11*EXP(-2044./TEMP)

RACM2_212 ACTP + NO → ACO3 + NO2 + HCHO; THERMAL A-FACT 2.90E-12 E/R -300.0

RACM2_235 ACTP + HO2 → 0.330 OP2 + 0.670 HO + 0.670 HCHO + 0.670 ACO3; THERMAL A-FACT 1.15E-13 E/R -1300.0

RACM2_267 ACTP + MO2 → 0.25 ROH + 1.50 HCHO + 0.50 ACO3 + 0.25 MOH + 0.50 HO2 + 0.125 ORA2; THERMAL A-FACT 7.50E-13 E/R -500.0

RACM2_299 ACTP + ACO3 → 0.50 MO2 + HCHO + 0.75 ORA2 + 0.50 ACO3; THERMAL A-FACT 7.51E-13 E/R -565.0

RACM2_324 ACTP + NO3 → ACO3 + NO2 + HCHO; THERMAL A-FACT 1.20E-12 E/R 0.0

SAPRC07<BP15> ACET + hv → 0.62*MECO3 + 1.38*MEO2 + 0.38*CO # 5.00e-1/SAPRC07<ACET-06>

CB_05_000 No Equivalent

RACM2_014 ACT + hv → ACO3 + MO2

SAPRC07<BP16> MEK + OH → 0.967*RO2C + 0.039*RO2XC + 0.039*zRNO3 + 0.376*xHO2 + 0.51*xMECO3 + 0.074*xRCO3 + 0.088*xHCHO + 0.504*xCCHO + 0.376*xRCHO + yROOH + 0.3*XC # 1.30e-12^2.00@25

CB_05_000 No Equivalent

RACM2_128 MEK + HO → MEKP + H2O; THERMAL A-FACT 1.30E-12 E/R 25.0

RACM2_202 MEKP + NO → 0.67 DCB1 + 0.67 HO2 + 0.33 HCHO + NO2; THERMAL A-FACT 4.00E-12 E/R 0.0

RACM2_236 MEKP + HO2 → OP2; THERMAL A-FACT 1.15E-13 E/R -1300.0

RACM2_268 MEKP + MO2 → 0.334 DCB1 + 0.834 HO2 + 0.25 MOH + HCHO + 0.25 ROH; THERMAL A-FACT 6.91E-13 E/R -508.0

RACM2_300 MEKP + ACO3 → 0.50 MO2 + 0.50 ORA2 + 0.334 DCB1 + 0.33 HO2 + 0.33 HCHO; THERMAL A-FACT 7.51E-13 E/R -565.0

RACM2_322 MEKP + NO3 → 0.67 DCB1 + 0.67 HO2 + 0.33 HCHO + NO2; THERMAL A-FACT 1.20E-12 E/R 0.0

RACM2_129 KET + HO → KETP + H2O; THERMAL A-FACT 2.80E-12 E/R - 10.0

RACM2_211 KETP + NO → 0.54 MGLY + 0.46 ALD + 0.23 ACO3 + 0.77 HO2 + 0.16 XO2 + NO2; THERMAL A-FACT 4.00E-12 E/R 0.0

RACM2_237 KETP + HO2 → OP2; THERMAL A-FACT 1.15E-13 E/R -1300.0

RACM2_269 KETP + MO2 → 0.50 DCB1 + HO2 + 0.25 MOH + 0.75 HCHO + 0.25 ROH; THERMAL A-FACT 6.91E-13 E/R -508.0

RACM2_298 KETP + ACO3 → 0.50 DCB1 + 0.50 HO2 + 0.50 ORA2 + 0.50 MO2; THERMAL A-FACT 7.51E-13 E/R -565.0

RACM2_323 KETP + NO3 → DCB1 + HO2 + NO2; THERMAL A-FACT 1.20E-12 E/R 0.0
RACM2_130 HKET + HO → HO2 + MGLY + H2O; THERMAL A-FACT 3.00E-12 E/R 0.0

SAPRC07<BP17> MEK + hν → MECO3 + RO2C + xHO2 + xCCHO + yROOH # 1.75e-1/SAPRC07<MEK-06>

CB_05_000 No Equivalent

RACM2_015 MEK + hν → ACO3 + 0.50 ETHP + 0.50 MO2

Methanol, Organic Acid and Organic Peroxide Reactions

SAPRC07<BP18> MEOH + OH → HCHO + HO2 # 2.85e-12@345

CB_05_R72 MEOH + OH → FORM + HO2 7.3E-12 @ 620

RACM2_073 MOH + HO → HO2 + HCHO; THERMAL A-FACT 2.85E-12 E/R 345.0

SAPRC07<BP19> FACD + OH → HO2 + CO2 # 4.50e-13

CB_05_R82 FACD + OH → HO2 4.00E-13

RACM2_147 ORA1 + HO → HO2 + CO2; THERMAL A-FACT 4.50E-13 E/R 0.

SAPRC07<BP20> AACD + OH → 0.509*MEO2 + 0.491*RO2C + 0.509*CO2 + 0.491*xHO2 + 0.491*xMGLY +
0.491*yROOH -0.491*XC # 4.20e-14@-855

CB_05_R97 AACD + OH → MEO2 4.0E-13 @ -200

RACM2_148 ORA2 + HO → 0.64 MO2 + 0.64 CO2 + 0.36 ORAP; THERMAL A-FACT 2.20E-14 E/R -1012.0

RACM2_344 ORAP + NO → NO2 + GLY + HO2; THERMAL A-FACT 4.00E-12 E/R 0.0

RACM2_345 ORAP + HO2 → OP2; THERMAL A-FACT 1.15E-13 E/R -1300.0

RACM2_346 ORAP + MO2 → HCHO + HO2 + GLY; THERMAL A-FACT 7.50E-13 E/R -500.0

RACM2_347 ORAP + ACO3 → MO2 + GLY; THERMAL A-FACT 7.51E-13 E/R -565.0

RACM2_348 ORAP + NO3 → NO2 + GLY + HO2; THERMAL A-FACT 1.20E-12 E/R 0.0

SAPRC07<BP21> PACD + OH → RO2C + xHO2 + 0.143*CO2 + 0.142*xCCHO + 0.4*xRCHO + 0.457*xBACL +
yROOH + -0.455*XC # 1.20e-12

CB_05_R95 PACD + OH → C2O3 4.0E-13 @ -200

RACM2_142 PAA + HO → 0.65 ACO3 + 0.35 HO + 0.35 HCHO + 0.35 XO2; THERMAL A-FACT 2.93E-12 E/R -190.0

SAPRC07<BP22> COOH + OH → 0.35*HCHO + 0.35*OH + 0.65*MEO2 # 2.90e-12@-190

CB_05_R70 MEPX+OH → 0.700*MEO2 + 0.300*XO2 + 0.300*HO2 3.8E-12 @ -200

RACM2_140 OP1 + HO → 0.65 MO2 + 0.35 HCHO + 0.35 HO; THERMAL A-FACT 2.90E-12 E/R -190.0

SAPRC07<BP23> COOH + hv → HCHO + HO2 + OH # 1.0/SAPRC07<COOH>

CB_05_R71 MEPX + hv → FORM + HO2 + OH 1.0 x <COOH_SAPRC99>

RACM2_029 OP1 + hv → HCHO + HO2 + HO

SAPRC07<BP24> ROOH + OH → 0.659*OH + 0.339*RO2C + 0.003*RO2XC + 0.003*zRNO3 + 0.659*RCHO + 0.045*xOH + 0.293*xHO2 + 0.046*xHCHO + 0.045*xCCHO + 0.168*xRCHO + 0.125*xMEK + 0.341*yROOH + - 0.135*XC # 6.78e-12

CB_05_R63 ROOH + OH → XO2 + 0.500*ALD2 + 0.500*ALDX 3.01E-12 @ -190

RACM2_141 OP2 + HO → 0.44 HC3P + 0.08 ALD + 0.49 HO + 0.07 XO2 + 0.41 KET; THERMAL A-FACT 3.40E-12 E/R -190.0

SAPRC07<BP25> ROOH + hv → RCHO + HO2 + OH # 1.0/SAPRC07<COOH>

CB_05_R64 ROOH + hv → OH + HO2 + 0.500*ALD2 + 0.500*ALDX 1.0 x <COOH_SAPRC99>

RACM2_030 OP2 + hv → ALD + HO2 + HO

SAPRC07<BP26> R6OOH + OH → 0.691*OH + 0.395*RO2C + 0.046*RO2XC + 0.046*zRNO3 + 0.691*PRD2 + 0.151*xOH + 0.112*xHO2 + 0.062*xCCHO + 0.235*xRCHO + 0.112*xPROD2 + 0.309*yR6OOH + 0.077*XC # 1.64e-11

CB_05_000 No Equivalent

RACM2_000 No Equivalent

SAPRC07<BP27> R6OOH + hv → OH + 0.142*HO2 + 0.782*RO2C + 0.077*RO2XC + 0.077*zRNO3 + 0.085*RCHO + 0.142*PRD2 + 0.782*xHO2 + 0.026*xCCHO + 0.058*xRCHO + 0.698*xPROD2 + 0.858*yR6OOH + 0.017*XC # 1.0/SAPRC07<COOH>

CB_05_000 No Equivalent

RACM2_000 No Equivalent

SAPRC07<BP28> RAOOH + OH → 0.045*OH + 0.192*HO2 + 0.63*RO2C + 0.132*RO2XC + 0.132*zRNO3 + 0.1*PRD2 + 0.093*MGLY + 0.045*IPRD + 0.032*xOH + 0.598*xHO2 + 0.594*xRCHO + 0.021*xMEK + 0.205*xMGLY + 0.021*xAFG1 + 0.021*xAFG2 + 0.763*yR6OOH + 3.413*XC # 1.08e-10

CB_05_000 No Equivalent

RACM2_000 No Equivalent

SAPRC07<BP29> RAOOH + hv → OH + HO2 + 0.5*GLY + 0.5*MGLY + 0.5*AFG1 + 0.5*AFG2 + 0.5*XC #
1.0/SAPRC07<COOH>
CB_05_000 No Equivalent
RACM2_000 No Equivalent

Dicarbonyl Reactions

SAPRC07<BP30> GLY + hv → 2*CO + 2*HO2 # 1.0/SAPRC07<GLY-07R>
CB_05_000 No Equivalent
RACM2_021 GLY + hv → 2.00 HO2 + 2.00 CO

SAPRC07<BP31> GLY + hv → HCHO + CO # 1.0/SAPRC07<GLY-07M>
CB_05_000 No Equivalent
RACM2_022 GLY + h{} → H2 + 2.00 CO
RACM2_023 GLY + h{} → HCHO + 2.00 CO

SAPRC07<BP32> GLY + OH → 0.63*HO2 + 1.26*CO + 0.37*RCO3 + -0.37*XC # 1.10e-11
CB_05_000 No Equivalent
RACM2_131 GLY + HO → HO2 + 2.0 CO + H2O; THERMAL A-FACT 1.10E-11 E/R 0.0

SAPRC07<BP33> GLY + NO3 → HNO3 + 0.63*HO2 + 1.26*CO + 0.37*RCO3 + -0.37*XC # 2.80e-12@2376
CB_05_000 No Equivalent
RACM2_152 GLY + NO3 → HNO3 + HO2 + 2.0 CO; THERMAL A-FACT 2.90E-12 E/R 1900.0

SAPRC07<BP34> MGLY + hv → HO2 + CO + MECO3 # 1.0/SAPRC07<MGLY-06>
CB_05_R140 MGLY + hv → C2O3 + HO2 + CO 1.0 x <MGLY_IUPAC05>
RACM2_024 MGLY + hv → ACO3 + HO2 + CO

SAPRC07<BP35> MGLY + OH → CO + MECO3 # 1.50e-11
CB_05_R139 OH + MGLY → XO2 + C2O3 1.7E-11
RACM2_132 MGLY + HO → ACO3 + CO + H2O; THERMAL A-FACT 9.26E-13 E/R -830.

SAPRC07<BP36> MGLY + NO3 → HNO3 + CO + MECO3 # 1.40e-12@1895
CB_05_000 No Equivalent
RACM2_153 MGLY + NO3 → HNO3 + ACO3 + CO; THERMAL A-FACT 3.76E-12 E/R 1900.0

SAPRC07<BP37> BACL → 2*MECO3 # 1.0/SAPRC07<BACL-07>

CB_05_000 No Equivalent

RACM2_000 No Equivalent

Aromatic Products

SAPRC07<BP38> CRES + OH → 0.2*BZO + 0.8*RO2C + 0.8*xHO2 + 0.8*yR6OOH + 0.25*xMGLY + 5.05*XC # 1.70e-12@-950

CB_05_R131 OH + CRES → 0.400*CRO + 0.600*XO2 + 0.600*HO2 + 0.300*OPEN 4.10E-11

RACM2_113 PHEN + HO → 0.07 CHO + 0.20 ADDC + 0.73 MCT + 0.73 HO2; THERMAL A-FACT 6.75E-12 E/R -405.

RACM2_114 CSL + HO → 0.07 CHO + 0.20 ADDC + 0.73 MCT + 0.73 HO2; THERMAL A-FACT 4.65E-11 E/R 0.0

RACM2_208 ADDC + NO → NO2 + HO2 + 0.68 GLY + 0.68 OP2 + 0.32 HKET; THERMAL A-FACT 2.70E-12 E/R -360.

RACM2_231 ADDC + HO2 → OP2; THERMAL A-FACT 3.75E-13 E/R -980.

RACM2_264 ADDC + MO2 → HCHO + 2.0 HO2 + 0.68 GLY + 0.32 HKET + 0.68 OP2; THERMAL A-FACT 3.56E-14 E/R -708.

RACM2_295 ADDC + ACO3 → MO2 + 2.0 HO2 + 0.68 GLY + 0.32 HKET + 0.68 OP2; THERMAL A-FACT 7.40E-13 E/R -708.

RACM2_319 ADDC + NO3 → NO2 + HO2 + 0.68 GLY + 0.68 OP2 + 0.32 HKET; THERMAL A-FACT 1.20E-12 E/R 0.0

RACM2_115 MCT + HO → MCTO; THERMAL A-FACT 2.05E-10 E/R 0.0

RACM2_117 MCTO + O3 → MCTP; THERMAL A-FACT 2.86E-13 E/R 0.0

RACM2_118 MCTO + NO2 → ONIT; THERMAL A-FACT 2.08E-12 E/R 0.0

RACM2_119 MCTP + NO → MCTO; THERMAL A-FACT 2.70E-12 E/R -360.

SAPRC07<BP39> CRES + NO3 → HNO3 + BZO + XC # 1.40e-11

CB_05_R132 CRES + NO3 → CRO + HNO3 2.20E-11

RACM2_116 MCT + NO3 → MCTO + HNO3; THERMAL A-FACT 2.01E-10 E/R 0.0

RACM2_123 MCTP + NO3 → MCTO + NO2; THERMAL A-FACT 1.20E-12 E/R 0.0

RACM2_155 PHEN + NO3 → 0.5 HNO3 + 0.4 CHO + 0.5 ADCN + 0.1 ADDC; THERMAL A-FACT 3.78E-12 E/R 0.0

RACM2_156 CSL + NO3 → 0.5 HNO3 + 0.4 CHO + 0.5 ADCN + 0.1 ADDC; THERMAL A-FACT 1.06E-12 E/R 0.0

RACM2_157 ADCN + NO → GLY + 2.00 NO2 + OP2; THERMAL A-FACT 2.70E-12 E/R -360.

RACM2_158 ADCN + NO3 → OP2 + GLY + 2.0 NO2; THERMAL A-FACT 1.20E-12 E/R 0.0

RACM2_159 ADCN + MO2 → HCHO + HO2 + 0.7 OP2 + 0.7 GLY + 0.7 NO2 + 0.3 ONIT; THERMAL A-FACT 3.56E-14 E/R 0.0

RACM2_160 ADCN + ACO3 → MO2 + HO2 + 0.7 OP2 + 0.7 GLY + 0.7 NO2 + 0.3 ONIT; THERMAL A-FACT 7.40E-13 E/R -708.

RACM2_161 ADCN + HO2 → OP2; THERMAL A-FACT 3.75E-13 E/R -980.

SAPRC07<BP40> NPHE + OH → BZO + XN # 3.50e-12

CB_05_000 No Equivalent

RACM2_000 No Equivalent

SAPRC07<BP41> NPHE → HONO + 6*XC # 1.50e-3/SAPRC07<NO2-06>

CB_05_000 No Equivalent

RACM2_000 No Equivalent

SAPRC07<BP42> NPHE → 6*XC + XN # 1.50e-2/SAPRC07<NO2-06>

CB_05_000 No Equivalent

RACM2_000 No Equivalent

SAPRC07<BP43> BALD + OH → BZCO3 # 1.20e-11

CB_05_000 No Equivalent

RACM2_109 BALD + HO → BALP + H2O; THERMAL A-FACT 5.32E-12 E/R -243.

RACM2_111 BAL1 + NO → BAL2 + NO2; THERMAL A-FACT 4.00E-12 E/R 0.0

RACM2_112 BAL2 + NO2 → ONIT; THERMAL A-FACT 2.00E-11 E/R 0.0

SAPRC07<BP44> BALD + hv → 7*XC # 6.00e-2/SAPRC07<BALD-06>

CB_05_000 No Equivalent

RACM2_028 BALD + hv → CHO + HO2 + CO

SAPRC07<BP45> BALD + NO3 → HNO3 + BZCO3 # 1.34e-12@1860

CB_05_000 No Equivalent

RACM2_000 No Equivalent

SAPRC07<BP46> AFG1 + OH → 0.217*MACO3 + 0.723*RO2C + 0.06*RO2XC + 0.06*zRNO3 + 0.521*xHO2 + 0.201*xMECO3 + 0.334*xCO + 0.407*xRCHO + 0.129*xMEK + 0.107*xGLY + 0.267*xMGLY + 0.783*yR6OOH + 0.284*XC # 7.40e-11

CB_05_000 No Equivalent

RACM2_138 DCB1 + HO → XO2 + ACO3 + ALD; THERMAL A-FACT 2.8E-11 E/R -175.

SAPRC07<BP47> AFG1 + O3 → 0.826*OH + 0.522*HO2 + 0.652*RO2C + 0.522*CO + 0.174*CO2 + 0.432*GLY + 0.568*MGLY + 0.652*xRCO3 + 0.652*xHCHO + 0.652*yR6OOH -0.872*XC # 9.66e-18

CB_05_R137 OPEN + O3 → 0.030*ALDX + 0.620*C2O3 + 0.700*FORM + 0.030*XO2 + 0.690*CO + 0.080*OH + 0.760*HO2 + 0.200*MGLY 5.4E-17 @ 500

RACM2_000 No Equivalent

SAPRC07<BP48> AFG1 + hv→ 1.023*HO2 + 0.173*MEO2 + 0.305*MECO3 + 0.5*MACO3 + 0.695*CO + 0.195*GLY + 0.305*MGLY + 0.217*XC # 1.0/SAPRC07<AFG1>

CB_05_R135 OPEN + hv → C2O3 + HO2 + CO 9.0 x <HCHO_R_SAPRC99>

RACM2_025 DCB1 + hv → 2.0 XO2 + 1.5 HO2 + 0.5 ACO3 + CO + 0.5 GLY + 0.5 MGLY

SAPRC07<BP49> AFG2 + OH → 0.217*MACO3 + 0.723*RO2C + 0.06*RO2XC + 0.06*zRNO3 + 0.521*xHO2 + 0.201*xMEOC3 + 0.334*xCO + 0.407*xRCHO + 0.129*xMEK + 0.107*xGLY + 0.267*xMGLY + 0.783*yR6OOH + 0.284*XC # 7.40e-11

CB_05_000 No Equivalent

RACM2_000 No Equivalent

SAPRC07<BP50> AFG2 + O3 → 0.826*OH + 0.522*HO2 + 0.652*RO2C + 0.522*CO + 0.174*CO2 + 0.432*GLY + 0.568*MGLY + 0.652*xRCO3 + 0.652*xHCHO + 0.652*yR6OOH -0.872*XC # 9.66e-18

CB_05_000 No Equivalent

RACM2_137 DCB2 + HO → XO2 + ACO3 + ALD; THERMAL A-FACT 2.8E-11 E/R -175.

SAPRC07<BP51> AFG2 + hv→ PRD2 + -1*XC # 1.0/SAPRC07<AFG1>

CB_05_000 No Equivalent

RACM2_026 DCB2 + hv → 2.0 XO2 + 1.5 HO2 + 0.5 ACO3 + CO + 0.5 GLY + 0.5 MGLY

RACM2_027 DCB3 + hv → ACO3 + HO2 + CO + OLIP

SAPRC07<BP52> AFG3 + OH → 0.206*MACO3 + 0.733*RO2C + 0.117*RO2XC + 0.117*zRNO3 + 0.561*xHO2 + 0.117*xMEOC3 + 0.114*xCO + 0.274*xGLY + 0.153*xMGLY + 0.019*xBACL + 0.195*xAFG1 + 0.195*xAFG2 + 0.231*xIPRD + 0.794*yR6OOH + 0.938*XC # 9.35e-11

CB_05_000 No Equivalent

RACM2_135 UALD + HO → 0.313 ACO3 + 0.687 UALP; THERMAL A-FACT 5.77E-12 E/R -533.0

RACM2_203 UALP + NO → NO2 + HO2 + 0.61 CO + 0.27 ALD + 0.03 HCHO + 0.18 GLY + 0.21 MGLY + 0.7 KET; THERMAL A-FACT 4.20E-12 E/R -181.

RACM2_226 UALP + HO2 → OP2; THERMAL A-FACT 7.70E-14 E/R -1298.

RACM2_251 UALP + MO2 → 0.773 HCHO + HO2 + 0.203 ALD + 0.525 KET + 0.305 CO + 0.105 MGLY + 0.135 GLY + 0.250 MOH + 0.250 ROH; THERMAL A-FACT 3.40E-14 E/R -221.
RACM2_282 UALP + ACO3 → 0.5 HO2 + 0.5 MO2 + 0.5 ORA2 + 0.27 ALD + 0.7 KET + 0.105 MGLY + 0.5 CO + 0.030 HCHO + 0.18 GLY; THERMAL A-FACT 8.40E-14 E/R -221.
RACM2_337 UALP + NO3 → NO2 + HO2 + 0.61 CO + 0.27 ALD + 0.03 HCHO + 0.18 GLY + 0.21 MGLY + 0.7 KET; THERMAL A-FACT 1.20E-12 E/R 0.0
RACM2_136 EPX + HO → XO2 + HO2 + ALD + CO; THERMAL A-FACT 2.8E-11 E/R -175.
RACM2_139 DCB3 + HO → ACO3 + CO + H2O; THERMAL A-FACT 1.00E-13 E/R 0.0

SAPRC07<BP53> AFG3 + O3 → 0.471*OH + 0.554*HO2 + 0.013*MECO3 + 0.258*RO2C + 0.007*RO2XC + 0.007*zRNO3 + 0.58*CO + 0.19*CO2 + 0.366*GLY + 0.184*MGLY + 0.35*AFG1 + 0.35*AFG2 + 0.139*AFG3 + 0.003*MACR + 0.004*MVK + 0.003*IPRD + 0.095*xHO2 + 0.163*xRCO3 + 0.163*xHCHO + 0.095*xMGLY + 0.264*yR6OOH + -0.575*XC # 1.43e-17

CB_05_000 No Equivalent

RACM2_179 UALD + O3 → 0.476 HO + 0.072 HO2 + 0.168 MO2 + 0.237 ACO3 + 0.1 XO2 + 0.243 CO + 0.218 HCHO + 0.062 ALD + 0.278 KET + 0.031 GLY + 0.653 MGLY + 0.044 ORA1; THERMAL A-FACT 1.66E-18 E/R 0.0
RACM2_182 EPX + O3 → 1.5 HO2 + 0.5 HO + 1.5 CO + 0.5 CO2 + GLY; THERMAL A-FACT 1.0E-16 E/R 0.0
RACM2_183 DCB3 + O3 → HO2 + 0.5 HO + 1.5 CO + 0.5 CO2 + 0.25 ORA1 + 0.25 ORA2 + 0.11 PAA + 2.48 MGLY; THERMAL A-FACT 8.0E-17 E/R 0.0

Methacrolein, Methyl Vinyl Ketone and Isoprene Products

SAPRC07<BP54> MACR + OH → 0.5*MACO3 + 0.5*RO2C + 0.5*xHO2 + 0.416*xCO + 0.084*xHCHO + 0.416*xMEK + 0.084*xMGLY + 0.5*yROOH + -0.416*XC # 8.00e-12@-380

CB_05_R145 OH + ISPD → 1.565*PAR + 0.167*FORM + 0.713*XO2 + 0.503*HO2 + 0.334*CO + 0.168*MGLY + 0.252*ALD2 + 0.210*C2O3 + 0.250*CXO3 + 0.120*ALDX 3.36E-11

RACM2_133 MACR + HO → MACP; THERMAL A-FACT 1.86E-11 E/R -176.

SAPRC07<BP55> MACR + O3 → 0.208*OH + 0.108*HO2 + 0.1*RO2C + 0.45*CO + 0.117*CO2 + 0.1*HCHO + 0.9*MGLY + 0.333*FACD + 0.1*xRCO3 + 0.1*xHCHO + 0.1*yROOH -0.1*XC # 1.40e-15@2100

CB_05_R146 O3 + ISPD → 0.114*C2O3 + 0.150*FORM + 0.850*MGLY + 0.154*HO2 + 0.268*OH + 0.064*XO2 + 0.020*ALD2 + 0.360*PAR + 0.225*CO 7.10E-18

RACM2_177 MACR + O3 → 0.10 ACO3 + 0.90 MGLY 0.32 HO2 + 0.22 CO + 0.19 HO + 0.45 ORA1; THERMAL A-FACT 1.36E-15 E/R 2112.0

SAPRC07<BP56> MACR + NO₃ → 0.5*MACO₃ + 0.5*RO₂C + 0.5*HNO₃ + 0.5*xHO₂ + 0.5*xCO + 0.5*yROOH + 1.5*XC + 0.5*XN # 1.50e-12@1815

CB_05_R147 NO₃ + ISPD → 0.357*ALDX + 0.282*FORM + 1.282*PAR + 0.925*HO₂ + 0.643*CO + 0.850*NTR + 0.075*CXO₃ + 0.075*XO₂ + 0.150*HNO₃ 1.00E-15 19

RACM2_167 MACR + NO₃ → 0.5 MACP + 0.5 HNO₃ + 0.5 CO + 0.5 HO₂ + 0.5 ONIT + 0.5 XO₂; THERMAL A-FACT 3.40E-12 E/R 0.0

SAPRC07<BP57> MACR + O₃P → RCHO + XC # 6.34e-12

CB_05_000 No Equivalent

RACM2_000 No Equivalent

SAPRC07<BP58> MACR + hv → 0.33*OH + 0.67*HO₂ + 0.34*MECO₃ + 0.33*MACO₃ + 0.33*RO₂C + 0.67*CO + 0.34*HCHO + 0.33*xMECO₃ + 0.33*xHCHO + 0.33*yROOH

1.0/SAPRC07<MACR-06>

CB_05_R148 ISPD + hv → 0.333*CO + 0.067*ALD2 + 0.900*FORM + 0.832*PAR + 1.033*HO₂ + 0.700*XO₂ + 0.967*C₂O₃ 0.0036 x <ACROLEIN_SAPRC99>

RACM2_018 MACR + hv → 0.66 HO₂ + 0.33 MACP + 0.67 CO + 0.67 HCHO + 0.67 ACO₃ + 0.34 HO + 0.34 XO₂

SAPRC07<BP59> MVK + OH → 0.975*RO₂C + 0.025*RO₂XC + 0.025*zRNO₃ + 0.3*xHO₂ + 0.675*xMECO₃ + 0.3*xHCHO + 0.675*xRCHO + 0.3*xMGLY + yROOH + -0.725*XC

2.60e-12@-610

CB_05_000 No Equivalent

RACM2_134 MVK + HO → MVKP; THERMAL A-FACT 2.60E-12 E/R -610.

RACM2_201 MVKP + NO → NO₂ + 0.7 ALD + 0.7 XO₂ + 0.7 ACO₃ + 0.3 HCHO + 0.3 MGLY + 0.3 HO₂; THERMAL A-FACT 4.20E-12 E/R -181.

RACM2_225 MVKP + HO₂ → OP2; THERMAL A-FACT 7.70E-14 E/R -1298.

RACM2_250 MVKP + MO₂ → 1.5 HCHO + HO₂ + 1.75 ALD + 1.16 XO₂ + 0.292 ORA2 + 0.500 MGLY + 1.16 ACO₃ + 0.250 MOH + 0.250 ROH; THERMAL A-FACT 3.40E-14 E/R -221.

RACM2_281 MVKP + ACO₃ → 0.5 HO₂ + 0.5 MO₂ + 1.083 ORA2 + 2.3 ALD + 1.16 XO₂ + HCHO + 0.5 MGLY + 1.16 ACO₃; THERMAL A-FACT 8.40E-14 E/R -221.

RACM2_327 MVKP + NO₃ → NO₂ + 0.7 ALD + 2.3 XO₂ + 2.3 ACO₃ + 0.3 HCHO + MGLY + HO₂; THERMAL A-FACT 1.20E-12 E/R 0.0

SAPRC07<BP60> MVK + O₃ → 0.164*OH + 0.064*HO₂ + 0.05*RO₂C + 0.05*xHO₂ + 0.475*CO + 0.124*CO₂ + 0.05*HCHO + 0.95*MGLY + 0.351*FACD + 0.05*xRCO₃ + 0.05*xHCHO + 0.05*yROOH + -0.05*XC # 8.50e-16@1520
CB_05_000 No Equivalent
RACM2_178 MVK + O₃ → 0.67 ORA1 + 0.11 HO + 0.11 HO₂ + 0.11 CO + 0.17 CO₂ + 0.95 MGLY + 0.05 HCHO + 0.05 HO + 0.05 XO₂ + 0.05 HCHO + 0.05 ACO₃; THERMAL A-FACT 7.51E-16 E/R 1520.

SAPRC07<BP62> MVK + O₃P → 0.45*RCHO + 0.55*MEK + 0.45*XC # 4.32e-12
CB_05_000 No Equivalent
RACM2_000 No Equivalent

SAPRC07<BP63> MVK + hv → 0.4*MEO₂ + 0.6*CO + 0.6*PRD2 + 0.4*MACO₃ + -2.2*XC # 1.0/SAPRC07<MVK-06>
CB_05_000 No Equivalent
RACM2_019 MVK + hv → 0.7 UALD 0.7 CO 0.3 MO₂ + 0.3 MACP

SAPRC07<BP64> IPRD + OH → 0.289*MACO₃ + 0.67*RO₂C + 0.67*xHO₂ + 0.041*RO₂XC + 0.041*zRNO₃ + 0.336*xCO + 0.055*xHCHO + 0.129*xCCHO + 0.013*xRCHO + 0.15*xMEK + 0.332*xPROD2 + 0.15*xGLY + 0.174*xMGLY + -0.504*XC + 0.711*yR6OOH # 6.19e-11
CB_05_000 No Equivalent
RACM2_000 No Equivalent

SAPRC07<BP65> IPRD + O₃ → 0.285*OH + 0.4*HO₂ + 0.048*RO₂C + 0.048*xRCO₃ + 0.498*CO + 0.14*CO₂ + 0.124*HCHO + 0.21*MEK + 0.023*GLY + 0.742*MGLY + 0.1*FACD + 0.372*PACD + 0.047*xCCHO + 0.001*xHCHO + 0.048*yR6OOH + -0.329*XC # 4.18e-18
CB_05_000 No Equivalent
RACM2_000 No Equivalent

SAPRC07<BP66> IPRD + NO₃ → 0.15*MACO₃ + 0.15*HNO₃ + 0.799*RO₂C + 0.799*xHO₂ + 0.051*RO₂XC + 0.051*zRNO₃ + 0.572*xCO + 0.227*xHCHO + 0.218*xRCHO + 0.008*xMGLY + 0.572*xRNO₃ + 0.85*yR6OOH + 0.278*XN + -0.815*XC # 1.00e-13
CB_05_000 No Equivalent
RACM2_000 No Equivalent

SAPRC07<BP67> IPRD + hv → 1.233*HO₂ + 0.467*MECO₃ + 0.3*RCO₃ + 1.233*CO + 0.3*HCHO + 0.467*CCHO + 0.233*MEK + -0.233*XC # 1.0/SAPRC07<MACR-06>
CB_05_000 No Equivalent
RACM2_000 No Equivalent

SAPRC07<BP68> PRD2 + OH → 0.472*HO2 + 0.379*xHO2 + 0.029*xMECO3 + 0.049*xRCO3 + 0.473*RO2C + 0.071*RO2XC + 0.071*zRNO3 + 0.002*HCHO + 0.211*xHCHO + 0.001*CCHO + 0.083*xCCHO + 0.143*RCHO + 0.402*xRCHO + 0.115*xMEK + 0.329*PRD2 + 0.007*xPROD2 + 0.528*yR6OOH + 0.877*XC # 1.55e-11

CB_05_000 No Equivalent
RACM2_000 No Equivalent

SAPRC07<BP69> PRD2 → 0.913*xHO2 + 0.4*MECO3 + 0.6*RCO3 + 1.59*RO2C + 0.087*RO2XC + 0.087*zRNO3 + 0.303*xHCHO + 0.163*xCCHO + 0.78*xRCHO + yR6OOH -0.091*XC # 4.86e-3/SAPRC07<MEK-06>

CB_05_000 No Equivalent
RACM2_000 No Equivalent

SAPRC07<BP70> RNO3 + OH → 0.189*HO2 + 0.305*xHO2 + 0.019*NO2 + 0.313*xNO2 + 0.976*RO2C + 0.175*RO2XC + 0.175*zRNO3 + 0.011*xHCHO + 0.429*xCCHO + 0.001*RCHO + 0.036*xRCHO + 0.004*xACET + 0.01*MEK + 0.17*xMEK + 0.008*PRD2 + 0.031*xPROD2 + 0.189*RNO3 + 0.305*xRNO3 + 0.157*yROOH + 0.636*yR6OOH + 0.174*XN + 0.04*XC # 7.20e-12

CB_05_R61 NTR + OH → HNO3 + HO2 + 0.330*FORM + 0.330*ALD2 + 0.330*ALDX – 0.660*PAR 5.9E-13 @ 360
RACM2_146 ONIT + HO → HC3P + NO2 + H2O; THERMAL A-FACT 5.31E-12 E/R 260.0

SAPRC07<BP71> RNO3 + hv → 0.344*HO2 + 0.554*xHO2 + NO2 + 0.721*RO2C + 0.102*RO2XC + 0.102*zRNO3 + 0.074*xHCHO + 0.061*xHCHO + 0.214*xCCHO + 0.23*xCCHO + 0.074*xRCHO + 0.063*xRCHO + 0.008*xACET + 0.124*MEK + 0.083*xMEK + 0.19*PRD2 + 0.261*xPROD2 + 0.066*yROOH + 0.591*yR6OOH + 0.396*XC # 1.0/SAPRC07<IC3ONO2>

CB_05_000 No Equivalent
RACM2_032 ONIT + hv → 0.20 ALD + 0.80 KET + HO2 + NO2

Reactions of Steady State Operators Used to Represent Radical or Product Formation in Peroxy Radical Reactions

SAPRC07<PO01> xHCHO → HCHO # 'RO2RO'

CB_05_000 No Equivalent
RACM2_000 No Equivalent

SAPRC07<PO02> xHCHO → XC # 'RO2XRO'

CB_05_000 No Equivalent
RACM2_000 No Equivalent

SAPRC07<PO03> xCCHO → CCHO # 'RO2RO'

CB_05_000 No Equivalent

RACM2_000 No Equivalent

SAPRC07<PO04> xCCHO → 2*XC # 'RO2XRO'

CB_05_000 No Equivalent

RACM2_000 No Equivalent

SAPRC07<PO05> xRCHO → RCHO # 'RO2RO'

CB_05_000 No Equivalent

RACM2_000 No Equivalent

SAPRC07<PO06> xRCHO → 3*XC # 'RO2XRO'

CB_05_000 No Equivalent

RACM2_000 No Equivalent

SAPRC07<PO07> xACET → ACET # 'RO2RO'

CB_05_000 No Equivalent

RACM2_000 No Equivalent

SAPRC07<PO08> xACET → 3*XC # 'RO2XRO'

CB_05_000 No Equivalent

RACM2_000 No Equivalent

SAPRC07<PO09> xMEK → MEK # 'RO2RO'

CB_05_000 No Equivalent

RACM2_000 No Equivalent

SAPRC07<PO10> xMEK → 4*XC # 'RO2XRO'

CB_05_000 No Equivalent

RACM2_000 No Equivalent

SAPRC07<PO11> xPROD2 → PRD2 # 'RO2RO'

CB_05_000 No Equivalent

RACM2_000 No Equivalent

SAPRC07<PO12> xPROD2 → 6*XC # 'RO2XRO'

CB_05_000 No Equivalent

RACM2_000 No Equivalent

SAPRC07<PO13> xGLY → GLY # 'RO2RO'

CB_05_000 No Equivalent

RACM2_000 No Equivalent

SAPRC07<PO14> xGLY → 2*XC # 'RO2XRO'

CB_05_000 No Equivalent

RACM2_000 No Equivalent

SAPRC07<PO15> xMGLY → MGLY # 'RO2RO'

CB_05_000 No Equivalent

RACM2_000 No Equivalent

SAPRC07<PO16> xMGLY → 3*XC # 'RO2XRO'

CB_05_000 No Equivalent

RACM2_000 No Equivalent

SAPRC07<PO17> xBACL → BACL # 'RO2RO'

CB_05_000 No Equivalent

RACM2_000 No Equivalent

SAPRC07<PO18> xBACL → 4*XC # 'RO2XRO'

CB_05_000 No Equivalent

RACM2_000 No Equivalent

SAPRC07<PO19> xBALD → BALD # 'RO2RO'

CB_05_000 No Equivalent

RACM2_000 No Equivalent

SAPRC07<PO20> xBALD → 7*XC # 'RO2XRO'

CB_05_000 No Equivalent

RACM2_000 No Equivalent

SAPRC07<PO21> xAFG1 → AFG1 # 'RO2RO'

CB_05_000 No Equivalent

RACM2_000 No Equivalent

SAPRC07<PO22> xAFG1 → 5*XC # 'RO2XRO'

CB_05_000 No Equivalent

RACM2_000 No Equivalent

SAPRC07<PO23> xAFG2 → AFG2 # 'RO2RO'

CB_05_000 No Equivalent

RACM2_000 No Equivalent

SAPRC07<PO24> xAFG2 → 5*XC # 'RO2XRO'

CB_05_000 No Equivalent

RACM2_000 No Equivalent

SAPRC07<PO25> xAFG3 → AFG3 # 'RO2RO'

CB_05_000 No Equivalent

RACM2_000 No Equivalent

SAPRC07<PO26> xAFG3 → 7*XC # 'RO2XRO'

CB_05_000 No Equivalent

RACM2_000 No Equivalent

SAPRC07<PO27> xMACR → MACR # 'RO2RO'

CB_05_000 No Equivalent

RACM2_000 No Equivalent

SAPRC07<PO28> xMACR → 4*XC # 'RO2XRO'

CB_05_000 No Equivalent

RACM2_000 No Equivalent

SAPRC07<PO29> xMVK → MVK # 'RO2RO'

CB_05_000 No Equivalent

RACM2_000 No Equivalent

SAPRC07<PO30> xMVK → 4*XC # 'RO2XRO'

CB_05_000 No Equivalent

RACM2_000 No Equivalent

SAPRC07<PO31> xIPRD → IPRD # 'RO2RO'

CB_05_000 No Equivalent

RACM2_000 No Equivalent

SAPRC07<PO32> xIPRD → 5*XC # 'RO2XRO'

CB_05_000 No Equivalent

RACM2_000 No Equivalent

SAPRC07<PO33> xRNO3 → RNO3 # 'RO2RO'

CB_05_R55 XO2N+NO → NTR 2.6E-12 @ -365

SAPRC07<PO34> xRNO3 → 6*XC + XN # 'RO2XRO'

CB_05_000 No Equivalent

RACM2_000 No Equivalent

SAPRC07<PO35> zRNO3 → RNO3 + -1*XN # 'RO2NO'

CB_05_000 No Equivalent

RACM2_000 No Equivalent

SAPRC07<PO36> zRNO3 → PRD2 + HO2 # 'RO22NN'

CB_05_000 No Equivalent

RACM2_000 No Equivalent

SAPRC07<PO37> zRNO3 → 6*XC # 'RO2XRO'

CB_05_000 No Equivalent

RACM2_000 No Equivalent

SAPRC07<PO38> yROOH → ROOH + -3*XC # 'RO2HO2'

CB_05_R57 XO2N+HO2 → ROOH 7.5E-13 @ -700

RACM2_000 No Equivalent

SAPRC07<PO39> $yROOH \rightarrow MEK + -4*XC \# 'RO2RO2M'$

CB_05_000 No Equivalent

RACM2_000 No Equivalent

SAPRC07<PO40> $yROOH \rightarrow # 'RO2RO'$

CB_05_000 No Equivalent

RACM2_000 No Equivalent

SAPRC07<PO41> $yR6OOH \rightarrow R6OOH + -6*XC \# 'RO2HO2'$

CB_05_000 No Equivalent

RACM2_000 No Equivalent

SAPRC07<PO42> $yR6OOH \rightarrow PRD2 + -6*XC \# 'RO2RO2M'$

CB_05_000 No Equivalent

RACM2_000 No Equivalent

SAPRC07<PO43> $yR6OOH \rightarrow # 'RO2RO'$

CB_05_000 No Equivalent

RACM2_000 No Equivalent

SAPRC07<PO44> $yRAOOH \rightarrow RAOOH + -8*XC \# 'RO2HO2'$

CB_05_000 No Equivalent

RACM2_000 No Equivalent

SAPRC07<PO45> $yRAOOH \rightarrow PRD2 + -6*XC \# 'RO2RO2M'$

CB_05_000 No Equivalent

RACM2_000 No Equivalent

SAPRC07<PO46> $yRAOOH \rightarrow # 'RO2RO'$

CB_05_000 No Equivalent

RACM2_000 No Equivalent

Methane Reaction

SAPRC07<BE01> CH4 + OH → MEO2 # 1.85e-12@1690

CB_05_R66 OH + CH4 → MEO2 2.45E-12 @ 1775

RACM2_071 CH4 + HO → MO2 + H2O; THERMAL A-FACT 1.85E-12 E/R 1690.0

Ethene Reactions

SAPRC07<BE02> ETHE + OH → RO2C + xHO2 + 1.61*xHCHO + 0.195*xCCHO + yROOH # 1.00e-28^4.50&8.80e-12^0.85&0.60&1.0

CB_05_R121 OH + ETH → XO2 + 1.560*FORM + 0.220*ALDX + HO2 1.0E-28^-0.8 & 8.8E-12

RACM2_080 ETE + HO → ETEP; TROE KO 1.00E-28 N 4.5 KINF 8.80E-12 M .85

RACM2_196 ETEP + NO → 1.6 HCHO + HO2 + NO2 + 0.2 ALD; THERMAL A-FACT 9.00E-12 E/R 0.0

RACM2_220 ETEP + HO2 → OP2; THERMAL A-FACT 1.90E-13 E/R -1300.0

RACM2_245 ETEP + MO2 → 1.95 HCHO + HO2 + 0.15 ALD + 0.250 MOH + 0.250 ETEG; THERMAL A-FACT 1.71E-13 E/R -708.0

RACM2_276 ETEP + ACO3 → 1.6 HCHO + 0.2 ALD + 0.5 HO2 + 0.5 MO2 + 0.5 ORA2; THERMAL A-FACT 9.48E-13 E/R -765.0

RACM2_311 ETEP + NO3 → 1.6 HCHO + HO2 + NO2 + 0.2 ALD; THERMAL A-FACT 1.20E-12 E/R 0.0

SAPRC07<BE03> ETHE + O3 → 0.16*OH + 0.16*HO2 + 0.51*CO + 0.12*CO2 + HCHO + 0.37*FACD # 9.14e-15@2580

CB_05_R122 O3 + ETH → FORM + 0.630*CO + 0.130*HO2 + 0.130*OH + 0.370*FACD 1.2E-14 @ 2630

RACM2_172 ETE + O3 → HCHO + 0.43 CO + 0.37 ORA1 + 0.26 HO2 + 0.13 H2 + 0.12 HO; THERMAL A-FACT 9.14E-15 E/R 2580.0

SAPRC07<BE04> ETHE + NO3 → RO2C + xHO2 + xRCHO + yROOH + -1*XC + XN # 3.30e-12^2.00@2880

CB_05_R123 NO3 + ETH → NO2 + XO2 + 2.0*FORM 3.3E-12 @ 2880

RACM2_162 ETE + NO3 → 0.80 OLNN + 0.20 OLND; THERMAL-T2 A-FACT 4.88E-18 E/R 2282.0

RACM2_213 OLNN + NO → ONIT + NO2 + HO2; THERMAL A-FACT 4.00E-12 E/R 0.0

RACM2_238 OLNN + HO2 → ONIT; THERMAL A-FACT 1.66E-13 E/R -1300.0

RACM2_270 OLNN + MO2 → HCHO + 2.00 HO2 + ONIT; THERMAL A-FACT 1.60E-13 E/R -708.0

RACM2_301 OLNN + ACO3 → ONIT + MO2 + HO2; THERMAL A-FACT 8.85E-13 E/R -765.0

RACM2_303 OLNN + OLNN → 2.00 ONIT + HO2; THERMAL A-FACT 7.00E-14 E/R -1000.0

RACM2_304 OLNN + OLND → 0.202 HCHO + 0.640 ALD + 0.149 KET + 0.500 HO2 + 0.500 NO2 + 1.50 ONIT; THERMAL A-FACT 4.25E-14 E/R -1000.0

RACM2_325 OLNN + NO3 → ONIT + NO2 + HO2; THERMAL A-FACT 1.20E-12 E/R 0.0

RACM2_214 OLND + NO → 0.287 HCHO + 1.24 ALD + 0.464 KET + 2.00 NO2; THERMAL A-FACT 4.00E-12 E/R 0.0
RACM2_239 OLND + HO2 → ONIT; THERMAL A-FACT 1.66E-13 E/R -1300.0
RACM2_271 OLND + MO2 → 0.965 HCHO + 0.500 HO2 + 0.930 ALD + 0.348 KET + 0.500 NO2 + 0.250 MOH + 0.25 ROH; THERMAL A-FACT 9.68E-14 E/R -708.0
RACM2_302 OLND + ACO3 → 0.287 HCHO + 1.24 ALD + 0.464 KET + 0.500 MO2 + 0.500 ORA2 + NO2; THERMAL A-FACT 5.37E-13 E/R -765.0
RACM2_305 OLND + OLND → 0.504 HCHO + 1.21 ALD + 0.285 KET + ONIT + NO2; THERMAL A-FACT 2.96E-14 E/R -1000.0
RACM2_326 OLND + NO3 → 0.287 HCHO + 1.24 ALD + 0.464 KET + 2.00 NO2; THERMAL A-FACT 1.20E-12 E/R 0.0

SAPRC07<BE05> ETHE + O3P → 0.8*HO2 + 0.51*MEO2 + 0.29*RO2C + 0.51*CO + 0.1*CCHO + 0.29*xHO2 + 0.278*xCO + 0.278*xHCHO + 0.012*xGLY + 0.29*yROOH + 0.2*XC # 1.07e-11@800

CB_05_R120 O + ETH → FORM + 1.700*HO2 + CO + 0.700*XO2 + 0.300*OH 1.04E-11 @ 792

RACM2_000 No Equivalent

Isoprene Reactions

SAPRC07<BE06> ISOP + OH → 0.986*RO2C + 0.093*RO2XC + 0.093*zRNO3 + 0.907*xHO2 + 0.624*xHCHO + 0.23*xMACR + 0.32*xMVK + 0.357*xIPRD + yR6OOH -0.167*XC # 2.54e-11@-410

CB_05_R142 OH + ISOP → 0.912*ISPD + 0.629*FORM + 0.991*XO2 + 0.912*HO2 + 0.088*XO2N 2.54E-11 @ -407.6
RACM2_084 ISO + HO → ISOP; THERMAL A-FACT 2.54E-11 E/R -410.

RACM2_199 ISOP + NO → 0.046 ISON + 0.954 NO2 + 0.954 HO2 + HCHO + 0.418 MACR + 0.582 MVK; THERMAL A-FACT 2.43E-12 E/R -360.

RACM2_223 ISOP + HO2 → ISHP; THERMAL A-FACT 2.05E-13 E/R -1300.

RACM2_248 ISOP + MO2 → 1.54 HCHO + HO2 + 0.305 MVK + 0.219 MACR + 0.250 MOH + 0.250 ROH; THERMAL A-FACT 3.40E-14 E/R -221.

RACM2_279 ISOP + ACO3 → 0.5 HO2 + 0.5 MO2 + 0.5 ORA2 + 1.048 HCHO + 0.219 MACR + 0.305 MVK; THERMAL A-FACT 8.40E-14 E/R -221.

RACM2_314 ISOP + NO3 → 0.438 MACR + 0.610 MVK + HO2 + NO2 + 1.05 HCHO; THERMAL A-FACT 1.20E-12 E/R 0.0

SAPRC07<BE07> ISOP + O3 → 0.266*OH + 0.066*HO2 + 0.192*RO2C + 0.008*RO2XC + 0.008*zRNO3 + 0.275*CO + 0.122*CO2 + 0.4*HCHO + 0.1*PRD2 + 0.39*MACR + 0.16*MVK + 0.15*IPRD + 0.204*FACD + 0.192*xMACO3 + 0.192*xHCHO + 0.2*yR6OOH + -0.559*XC # 7.86e-15@1912

CB_05_R143 O3 + ISOP → 0.650*ISPD + 0.600*FORM + 0.200*XO2 + 0.066*HO2 + 0.266*OH + 0.200*CXO3 + 0.150*ALDX + 0.350*PAR + 0.066*CO 7.86E-15 @ 1912

RACM2_176 ISO + O3 → 0.58 HCHO + 0.461 MACR + 0.189 MVK + 0.28 ORA1 + 0.25 HO + 0.25 HO2 + 0.14 CO + 0.1 ACO3 + 0.08 MO2 + 0.09 H2O2 + 0.1 MACP; THERMAL A-FACT 7.86E-15 E/R 1913.

SAPRC07<BE08> ISOP + NO3 → 0.936*RO2C + 0.064*RO2XC + 0.064*zRNO3 + 0.749*xHO2 + 0.187*xNO2 + 0.936*xIPRD + yR6OOH + -0.064*XC + 0.813*XN # 3.03e-12@448

CB_05_R144 NO3 + ISOP → 0.200*ISPD + 0.800*NTR + XO2 + 0.800*HO2 + 0.200*NO2 + 0.800*ALDX + 2.400*PAR 3.03E-12 @ 448 19

RACM2_166 ISO + NO3 → ISON; THERMAL A-FACT 3.03E-12 E/R 446.

SAPRC07<BE09> ISOP + O3P → 0.25*MEO2 + 0.24*RO2C + 0.01*RO2XC + 0.01*zRNO3 + 0.75*PRD2 + 0.24*xMACO3 + 0.24*xHCHO + 0.25*yR6OOH + -1.01*XC # 3.50e-11

CB_05_R141 O + ISOP → 0.750*ISPD + 0.500*FORM + 0.250*XO2 + 0.250*HO2 + 0.250*CXO3 + 0.250*PAR 3.60E-11

RACM2_000 No Equivalent

Acetylene Reactions

SAPRC07<BE10> ACYE + OH → 0.7*OH + 0.3*HO2 + 0.3*CO + 0.7*GLY + 0.3*FACD # 5.50e-30^-2.00&8.30e-13&0.60&1.0

CB_05_000 No Equivalent

RACM2_076 ACE + HO → 0.350 ORA1 + 0.350 CO + 0.650 GLY + 0.650 HO + 0.350 HO2; TROE KO 5.50E-30 N 0.0 KINF 8.30E-13 M -2.0

SAPRC07<BE11> ACYE + O3 → 0.5*OH + 1.5*HO2 + 1.5*CO + 0.5*CO2 # 1.00e-14@4100

CB_05_000 No Equivalent

RACM2_000 No Equivalent

Benzene Reaction

SAPRC07<BE12> BENZ + OH → 0.116*OH + 0.29*RO2C + 0.29*xHO2 + 0.024*RO2XC + 0.024*zRNO3 + 0.57*HO2 + 0.57*CRES + 0.116*AFG3 + 0.29*xGLY + 0.029*xAFG1 + 0.261*xAFG2 + 0.314*yRAOOH + -0.976*XC # 2.33e-12@193

CB_05_000 No Equivalent

RACM2_093 BEN + HO → 0.352 BENP + 0.118 UALD + 0.530 PHEN + 0.648 HO2

THERMAL A-FACT 2.33E-12 E/R 193.0

RACM2_206 BENP + NO → 0.082 ONIT + 0.918 HO2 + 0.459 UALD + 0.918 NO2 + 0.459 OLI + 0.918 GLY; THERMAL A-FACT 2.54E-12 E/R -360.

RACM2_229 BENP + HO2 → OP2; THERMAL A-FACT 2.91E-13 E/R -1300.

RACM2_254 BENP + MO2 → HCHO + 1.6 HO2 + 0.600 GLY + 0.300 OLI + 0.7 UALD; THERMAL A-FACT 3.56E-14 E/R -708.

RACM2_285 BENP + ACO3 → MO2 + 0.60 HO2 + 0.600 GLY + 0.700 UALD + 0.30 OLI
THERMAL A-FACT 7.40E-13 E/R -765.

RACM2_317 BENP + NO3 → HO2 + GLY + UALD + NO2; THERMAL A-FACT 1.20E-12 E/R 0.0

Alkane Reactions

SAPRC07<BL01> ALK1 + OH → xHO2 + RO2C + xCCHO + yROOH # 1.34e-12^2.00@499

CB_05_R155 OH + ETHA → 0.991*ALD2 + 0.991*XO2 + 0.009*XO2N + HO2 8.7E-12 @ 1070

RACM2_072 ETH + HO → ETHP + H2O; THERMAL A-FACT 6.90E-12 E/R 1000.0

RACM2_192 ETHP + NO → ACD + HO2 + NO2; THERMAL A-FACT 2.60E-12 E/R -365.0

RACM2_216 ETHP + HO2 → OP2; THERMAL A-FACT 7.50E-13 E/R -700.0

RACM2_241 ETHP + MO2 → 0.75 HCHO + HO2 0.75 ACD + 0.250 MOH + 0.250 EOH; THERMAL A-FACT 1.18E-13 E/R -158.0

RACM2_272 ETHP + ACO3 → ACD + 0.500 HO2 + 0.5 MO2 + 0.5 ORA2; THERMAL A-FACT 1.03E-12 E/R -211.0

RACM2_307 ETHP + NO3 → ACD + HO2 + NO2; THERMAL A-FACT 1.20E-12 E/R 0.0

SAPRC07<BL02> ALK2 + OH → 0.965*xHO2 + 0.965*RO2C + 0.035*RO2XC + 0.035*zRNO3 + 0.261*xRCHO + 0.704*xACET + yROOH + -0.105*XC # 1.49e-12^2.00@87

CB_05_R112 PAR + OH → 0.870*XO2 + 0.130*XO2N + 0.110*HO2 + 0.060*ALD2 - 0.110*PAR + 0.760*ROR + 0.050*ALDX 8.10E-13

RACM2_077 HC3 + HO → HC3P; THERMAL A-FACT 7.68E-12 E/R 370.0

RACM2_193 HC3P + NO → 0.047 HCHO + 0.233 ALD + 0.623 ACT + 0.063 GLY + 0.742 HO2 + 0.150 MO2 + 0.048 ETHP + 0.048 XO2 + 0.059 ONIT + 0.941 NO2; THERMAL A-FACT 4.00E-12 E/R 0.0

RACM2_217 HC3P + HO2 → OP2; THERMAL A-FACT 1.66E-13 E/R -1300.0
RACM2_242 HC3P + MO2 → 0.827 HCHO + 0.894 HO2 + 0.198 ALD + 0.497 KET + 0.080 MO2 + 0.250 MOH + 0.026
XO2 + 0.050 GLY + 0.026 ETHP + 0.250 ROH; THERMAL A-FACT 9.46E-14 E/R -431.0
RACM2_273 HC3P + ACO3 → 0.273 ALD + 0.662 KET + 0.394 HO2 + 0.580 MO2 + 0.500 ORA2 + 0.130 HCHO +
0.026 ETHP + 0.026 XO2 + 0.067 GLY; THERMAL A-FACT 6.90E-13 E/R -460.0
RACM2_308 HC3P + NO3 → 0.050 HCHO + 0.248 ALD + 0.662 KET + 0.067 GLY + 0.789 HO2 + 0.159 MO2 + 0.051
ETHP + 0.051 XO2 + NO2; THERMAL A-FACT 1.20E-12 E/R 0.0

SAPRC07<BL03> ALK3 + OH → 0.695*xHO2 + 0.236*xTBUO + 1.253*RO2C + 0.07*RO2XC + 0.07*zRNO3 +
0.026*xHCHO + 0.445*xCCHO + 0.122*xRCHO + 0.024*xACET + 0.332*xMEK + 0.983*yROOH + 0.017*yR6OOH + -
0.046*XC # 1.51e-12@-126

CB_05_000 No Equivalent

RACM2_078 HC5 + HO → HC5P + H2O; THERMAL A-FACT 1.01E-11 E/R 245.0
RACM2_194 HC5P + NO → 0.021 HCHO + 0.211 ALD + 0.500 KET + 0.599 HO2 + 0.031 MO2 + 0.245 ETHP + 0.334
XO2 + 0.124 ONIT + 0.876 NO2 + 0.122 MEK + 0.100 ACT; THERMAL A-FACT 4.00E-12 E/R 0.0
RACM2_218 HC5P + HO2 → OP2; THERMAL A-FACT 1.66E-13 E/R -1300.0
RACM2_243 HC5P + MO2 → 0.777 HCHO + 0.842 HO2 + 0.251 ALD + 0.618 KET + 0.140 ETHP + 0.191 XO2 + 0.018
MO2 + 0.250 MOH + 0.250 ROH; THERMAL A-FACT 1.00E-13 E/R -467.0
RACM2_274 HC5P + ACO3 → 0.381 ALD + 0.824 KET + 0.342 HO2 + 0.518 MO2 + 0.500 ORA2 + 0.042 HCHO +
0.140 ETHP + 0.191 XO2; THERMAL A-FACT 5.59E-13 E/R -522.0
RACM2_309 HC5P + NO3 → 0.024 HCHO + 0.241 ALD + 0.824 KET + 0.684 HO2 + 0.035 MO2 + 0.280 ETHP + 0.381
XO2 + NO2; THERMAL A-FACT 1.20E-12 E/R 0.0

SAPRC07<BL04> ALK4 + OH → 0.83*xHO2 + 0.01*xMEO2 + 0.011*xMECO3 + 1.763*RO2C + 0.149*RO2XC +
0.149*zRNO3 + 0.002*xCO + 0.029*xHCHO + 0.438*xCCHO + 0.236*xRCHO + 0.426*xACET + 0.106*xMEK +
0.146*xPROD2 + yR6OOH -0.119*XC # 3.75e-12@-44

CB_05_000 No Equivalent

RACM2_000 No Equivalent

SAPRC07<BL05> ALK5 + OH → 0.647*xHO2 + 1.605*RO2C + 0.353*RO2XC + 0.353*zRNO3 + 0.04*xHCHO +
0.106*xCCHO + 0.209*xRCHO + 0.071*xACET + 0.086*xMEK + 0.407*xPROD2 + yR6OOH + 2.004*XC # 2.70e-12@-
374

CB_05_000 No Equivalent

RACM2_079 HC8 + HO → 0.951 HC8P + 0.025 ALD + 0.024 HKET + 0.049 HO2 + H2O; THERMAL A-FACT 2.82E-11
E/R 273.0

RACM2_195 HC8P + NO → 0.150 ALD + 0.642 KET + 0.133 ETPH + 0.261 ONIT + 0.739 NO₂ + 0.606 HO₂ + 0.416 XO₂; THERMAL A-FACT 4.00E-12 E/R 0.0
 RACM2_219 HC8P + HO₂ → OP2; THERMAL A-FACT 1.66E-13 E/R -1300.0
 RACM2_244 HC8P + MO₂ → 0.750 HCHO + 0.910 HO₂ + 0.197 ALD + 0.652 KET + 0.281 XO₂ + 0.090 ETPH + 0.250 MOH + 0.250 ROH; THERMAL A-FACT 4.34E-14 E/R -633.
 RACM2_275 HC8P + ACO₃ → 0.217 ALD + 0.642 KET + 0.303 HO₂ + 0.500 MO₂ + 0.495 ORA2 + 0.067 ETPH + 0.208 X_O₂; THERMAL A-FACT 2.47E-13 E/R -683.
 RACM2_310 HC8P + NO₃ → 0.203 ALD + 0.869 KET + 0.180 ETPH + NO₂ + 0.820 HO₂ + 0.563 X_O₂; THERMAL A-FACT 1.20E-12 E/R 0.0

Alkene Reactions

SAPRC07<BL06> OLE1 + OH → 0.904*xHO₂ + 0.001*xMEO₂ + 1.138*RO₂C + 0.095*RO₂XC + 0.095*zRNO₃ + 0.7*xHCHO + 0.301*xCCHO + 0.47*xRCHO + 0.005*xACET + 0.026*xMACR + 0.008*xMVK + 0.006*xIPRD + 0.119*xPROD2 + 0.413*yROOH + 0.587*yR6OOH + 0.822*XC # 6.18e-12@-501
 CB_05_R117 OH + OLE → 0.800*FORM + 0.330*ALD2 + 0.620*ALDX + 0.800*XO₂ + 0.950*HO₂ – 0.700*PAR 3.20E-11
 RACM2_081 OLTP + HO → OLTP; THERMAL A-FACT 5.72E-12 E/R -500.0
 RACM2_197 OLTP + NO → 0.94 ALD + HCHO + HO₂ + NO₂ + 0.06 KET; THERMAL A-FACT 4.00E-12 E/R 0.0
 RACM2_221 OLTP + HO₂ → OP2; THERMAL A-FACT 1.66E-13 E/R -1300.0
 RACM2_246 OLTP + MO₂ → 1.50 HCHO + HO₂ + 0.705 ALD + 0.045 KET + 0.250 MOH + 0.250 ROH; THERMAL A-FACT 1.46E-13 E/R -708.0
 RACM2_277 OLTP + ACO₃ → 0.940 ALD + HCHO + 0.500 HO₂ + 0.500 MO₂ + 0.500 ORA2 + 0.060 KET; THERMAL A-FACT 8.11E-13 E/R -765.0
 RACM2_312 OLTP + NO₃ → 0.94 ALD + HCHO + HO₂ + NO₂ + 0.06 KET; THERMAL A-FACT 1.20E-12 E/R 0.0

SAPRC07<BL07> OLE1 + O₃ → 0.116*HO₂ + 0.04*xHO₂ + 0.193*OH + 0.104*MEO₂ + 0.063*RO₂C + 0.004*RO₂XC + 0.004*zRNO₃ + 0.368*CO + 0.125*CO₂ + 0.5*HCHO + 0.147*CCHO + 0.007*xCCHO + 0.353*RCHO + 0.031*xRCHO + 0.002*xACET + 0.006*MEK + 0.185*FACD + 0.022*AACD + 0.112*PACD + 0.189*PRD2 + 0.007*yROOH + 0.037*yR6OOH + 0.69*XC # 3.15e-15@1701
 CB_05_R118 O₃ + OLE → 0.180*ALD2 + 0.740*FORM + 0.320*ALDX + 0.220*XO₂ + 0.100*OH + 0.330*CO + 0.440*HO₂ – PAR 6.5E-15 @ 1900
 RACM2_173 OLTP + O₃ → 0.64 HCHO + 0.44 ALD + 0.37 CO + 0.14 ORA1 + 0.10 ORA2 + 0.25 HO₂ + 0.40 HO + 0.03 KET + 0.03 KETP + 0.06 CH₄ + 0.05 H₂ + 0.03 ETH + 0.006 H₂O₂ + 0.19 MO₂ + 0.10 ETPH; THERMAL A-FACT 4.33E-15 E/R 1800.0

SAPRC07<BL08> OLE1 + NO3 → 0.824*xHO2 + 1.312*RO2C + 0.176*RO2XC + 0.176*zRNO3 + 0.009*xCCHO + 0.002*xRCHO + 0.024*xACET + 0.546*xRNO3 + 0.413*yROOH + 0.587*yR6OOH + 0.454*XN + 0.572*XC # 4.73e-13@1047

CB_05_R119 NO3 + OLE → NO2 + FORM + 0.910*XO2 + 0.090*XO2N + 0.560*ALDX + 0.350*ALD2 – PAR 7E-13 @ 2160

RACM2_163 OLT + NO3 → 0.43 OLNN + 0.57 OLND; THERMAL A-FACT 1.79E-13 E/R 450.0

SAPRC07<BL09> OLE1 + O3P → 0.45*RCHO + 0.437*MEK + 0.113*PRD2 + 1.224*XC # 1.49e-11@326

CB_05_R116 O + OLE → 0.200*ALD2 + 0.300*ALDX + 0.300*HO2 + 0.200*XO2 + 0.200*CO + 0.200*FORM + 0.010*XO2N + 0.200*PAR + 0.100*OH 1.E-11 @ 280

RACM2_000 No Equivalent

SAPRC07<BL10> OLE2 + OH → 0.914*xHO2 + 0.966*RO2C + 0.086*RO2XC + 0.086*zRNO3 + 0.209*xHCHO + 0.788*xCCHO + 0.481*xRCHO + 0.136*xACET + 0.076*xMEK + 0.027*xMACR + 0.002*xMVK + 0.037*xIPRD + 0.022*xPROD2 + 0.357*yROOH + 0.643*yR6OOH + 0.111*XC # 1.26e-11@-488

CB_05_R125 IOLE + OH → 1.300*ALD2 + 0.700*ALDX + HO2 + XO2 1.0E-11 @ -550

RACM2_082 OLI + HO → OLIP; THERMAL A-FACT 1.33E-11 E/R -500.0

RACM2_083 DIEN + HO → OLIP; THERMAL A-FACT 1.48E-11 E/R -448.0

RACM2_198 OLIP + NO → HO2 + 1.71 ALD + 0.29 KET + NO2; THERMAL A-FACT 4.00E-12 E/R 0.0

RACM2_222 OLIP + HO2 → OP2; THERMAL A-FACT 1.66E-13 E/R -1300.0

RACM2_247 OLIP + MO2 → 0.750 HCHO + HO2 + 1.28 ALD + 0.218 KET + 0.250 MOH + 0.250 ROH; THERMAL A-FACT 9.18E-14 E/R -708.0

RACM2_278 OLIP + AC03 → 1.71 ALD + 0.500 HO2 + 0.500 MO2 + 0.290 KET + 0.500 ORA2; THERMAL A-FACT 5.09E-13 E/R -765.0

RACM2_313 OLIP + NO3 → HO2 + 1.71 ALD 0.29 KET + NO2; THERMAL A-FACT 1.20E-12 E/R 0.0

SAPRC07<BL11> OLE2 + O3 → 0.093*HO2 + 0.039*xHO2 + 0.423*OH + 0.29*MEO2 + 0.147*xMEOC3 + 0.008*xRCO3 + 0.2*RO2C + 0.003*RO2XC + 0.003*zRNO3 + 0.297*CO + 0.162*CO2 + 0.152*HCHO + 0.108*xHCHO + 0.428*CCHO + 0.067*xCCHO + 0.315*RCHO + 0.018*xRCHO + 0.048*ACET + 0.031*MEK + 0.001*xMEK + 0.033*FACD + 0.061*AACD + 0.222*PACD + 0.028*MACR + 0.021*MVK + 0.042*PRD2 + 0.069*yROOH + 0.128*yR6OOH + 0.125*XC # 8.14e-15@1255

CB_05_R126 IOLE + O3 → 0.650*ALD2 + 0.350*ALDX + 0.250*FORM + 0.250*CO + 0.500*O + 0.500*OH + 0.500*HO2 8.4E-15 @ 1100

RACM2_174 OLI + O3 → 0.02 HCHO + 0.99 ALD + 0.16 KET + 0.30 CO + 0.011 H2O2 + 0.14 ORA2 + 0.07 CH4 + 0.22 HO2 + 0.63 HO + 0.23 MO2 + 0.12 KETP + 0.06 ETH + 0.18 ETPH; THERMAL A-FACT 4.40E-15 E/R 845.0

RACM2_175 DIEN + O3 → 0.90 HCHO + 0.39 MACR + 0.36 CO + 0.15 ORA1 + 0.09 O3P + 0.30 HO2 + 0.35 OLT +
0.28 HO + 0.05 H2 + 0.15 ACO3 + 0.03 MO2 + 0.02 KETP + 0.13 XO2 + 0.001 H2O2; THERMAL A-FACT 1.34E-14 E/R
2283.0

SAPRC07<BL12> OLE2 + NO3 → 0.423*xHO2 + 0.409*xNO2 + 0.033*xMEO2 + 1.185*RO2C + 0.136*RO2XC + 0.136*zRNO3 + 0.074*xHCHO + 0.546*xCCHO + 0.154*xRCHO + 0.11*xACET + 0.002*xMEK + 0.026*xMVK + 0.007*xIPRD + 0.322*xRNO3 + 0.357*yROOH + 0.643*yR6OOH + 0.269*XN + 0.114*XC # 2.20e-13@-382

CB_05_R127 IOLE + NO3 → 1.180*ALD2 + 0.640*ALDX + HO2 + NO2 9.6E-13 @ 270

RACM2_164 OLI + NO3 → 0.11 OLNN + 0.89 OLND; THERMAL A-FACT 8.64E-13 E/R -450.

RACM2_165 DIEN + NO3 → 0.90 OLNN + 0.10 OLND + 0.90 MACR; THERMAL A-FACT 1.00E-13 E/R 0.0

SAPRC07<BL13> OLE2 + O3P → 0.014*HO2 + 0.007*xHO2 + 0.007*xMACO3 + 0.013*RO2C + 0.001*RO2XC + 0.001*zRNO3 + 0.006*xCO + 0.074*RCHO + 0.709*MEK + 0.006*xMACR + 0.202*PRD2 + 0.014*yROOH + 0.666*XC # 1.43e-11@-111

CB_05_R124 IOLE + O → 1.240*ALD2 + 0.660*ALDX + 0.100*HO2 + 0.100*XO2 + 0.100*CO + 0.100*PAR 2.3E-11

RACM2_000 No Equivalent

Aromatic Reactions

SAPRC07<BL14> ARO1 + OH → 0.166*HO2 + 0.482*xHO2 + 0.284*OH + 0.482*RO2C + 0.068*RO2XC + 0.068*zRNO3 + 0.218*xGLY + 0.138*xMGLY + 0.166*CRES + 0.049*xBALD + 0.164*xAFG1 + 0.193*xAFG2 + 0.284*AFG3 + 0.077*xPROD2 + 0.403*yRAOOH + 0.147*yR6OOH + 0.002*XC # 6.15e-12

CB_05_R128 TOL + OH → 0.440*HO2 + 0.080*XO2 + 0.360*CRES + 0.560*TO2 1.8E-12 @ -355

RACM2_094 TOL + HO → 0.060 TLP1 + 0.890 TR2 + 0.050 CSL + 0.050 HO2; THERMAL A-FACT 1.81E-12 E/R -354.

RACM2_095 TLP1 + NO → NO2 + BALD; THERMAL A-FACT 4.00E-12 E/R 0.0

RACM2_256 TLP1 + MO2 → HCHO + HO2 + BALD; THERMAL A-FACT 3.56E-14 E/R -708.

RACM2_287 TLP1 + ACO3 → MO2 + BALD; THERMAL A-FACT 7.40E-13 E/R -765.

RACM2_329 TLP1 + NO3 → NO2 + BALD; THERMAL A-FACT 1.20E-12 E/R 0.0

RACM2_096 TR2 → 0.280 DCB2 + 0.280 EPX + 0.010 CSL + 0.280 TOLP + 0.150 PER1 + 0.290 HO2 + 0.280 HO; THERMAL A-FACT 1.00E+03 E/R 0.0

RACM2_097 TOLP → 0.490 DCB2 + 0.010 HO2 + 0.010 CSL + 0.490 HO + 0.500 PER1; THERMAL A-FACT 1.00E+03 E/R 0.0

RACM2_098 TOLP + NO → 0.95 DCB2 + 0.95 NO2 + 0.95 HO2 + 0.050 ONIT; THERMAL A-FACT 2.70E-12 E/R -360.

RACM2_255 TOLP + MO2 → HCHO + 2.0 HO2 + 0.271 GLY + DCB2; THERMAL A-FACT 3.56E-14 E/R -708.

RACM2_286 TOLP + ACO3 → DCB2 + HO2 + MO2; THERMAL A-FACT 7.40E-13 E/R -765.

RACM2_330 TOLP + NO3 → DCB2 + NO2 + HO2; THERMAL A-FACT 1.20E-12 E/R 0.0

RACM2_099 PER1 + NO → 0.95 DCB1 + 0.95 NO2 + 0.95 MGLY + 0.95 HO2 + 0.050 ONIT; THERMAL A-FACT 2.70E-12 E/R -360.

RACM2_257 PER1 + MO2 → HCHO + 2.0 HO2 + MGLY + DCB1; THERMAL A-FACT 3.56E-14 E/R -708.

RACM2_288 PER1 + ACO3 → DCB1 + MO2 + MGLY + HO2; THERMAL A-FACT 7.40E-13 E/R -765.

RACM2_331 PER1 + NO3 → DCB1 + NO2 + MGLY + HO2; THERMAL A-FACT 1.20E-12 E/R 0.0

SAPRC07<BL15> ARO2 + OH → 0.108*HO2 + 0.58*xHO2 + 0.202*OH + 0.58*RO2C + 0.11*RO2XC + 0.11*zRNO3 + 0.116*xGLY + 0.286*xMGLY + 0.104*xBACL + 0.108*CRES + 0.039*xBALD + 0.217*xAFG1 + 0.21*xAFG2 + 0.202*AFG3 + 0.08*xAFG3 + 0.035*xPROD2 + 0.089*yR6OOH + 0.601*yRAOOH + 1.486*XC # 2.57e-11

CB_05_R138 OH + XYL → 0.700*HO2 + 0.500*XO2 + 0.200*CRES + 0.800*MGLY + 1.100*PAR + 0.300*TO2 1.7E-11
@ -116 17

RACM2_100 XYO + HO → 0.060 XYL1 + 0.890 XY02 + 0.050 CSL + 0.050 HO2; THERMAL A-FACT 1.37E-11 E/R 0.0

RACM2_101 XYL + HO → 0.060 XYL1 + 0.890 XY2 + 0.050 CSL + 0.050 HO2; THERMAL A-FACT 2.13E-11 E/R 0.0

RACM2_102 XYL1 + NO → NO2 + BALD; THERMAL A-FACT 4.00E-12 E/R 0.0

RACM2_259 XYL1 + MO2 → HCHO + HO2 + BALD; THERMAL A-FACT 3.56E-14 E/R -708.

RACM2_293 XYL1 + ACO3 → MO2 + BALD; THERMAL A-FACT 7.40E-13 E/R -765.

RACM2_332 XYL1 + NO3 → NO2 + BALD; THERMAL A-FACT 1.20E-12 E/R 0.0

RACM2_103 XY2 → 0.224 DCB2 + 0.840 EPX + 0.010 CSL + 0.308 XYLP + 0.150 PER2 + 0.308 HO2 + 0.308 HO; THERMAL A-FACT 1.00E+03 E/R 0.0

RACM2_104 XY02 → 0.224 DCB2 + 0.840 EPX + 0.010 CSL + 0.308 XYOP + 0.150 PER2 + 0.308 HO2 + 0.308 HO; THERMAL A-FACT 1.00E+03 E/R 0.0

RACM2_105 XYLP → 0.490 DCB2 + 0.010 HO2 + 0.010 CSL + 0.490 HO + 0.500 PER2; THERMAL A-FACT 1.00E+03 E/R 0.0

RACM2_106 XYOP → 0.490 DCB2 + 0.010 HO2 + 0.010 CSL + 0.490 HO + 0.500 PER2; THERMAL A-FACT 1.00E+03 E/R 0.0

RACM2_207 XYOP + NO → 0.95 HO2 + 0.350 GLY + 0.600 MGLY + 0.700 DCB1 + 0.073 DCB2 + 0.177 DCB3 + 0.05 ONIT + 0.95 NO2; THERMAL A-FACT 2.70E-12 E/R -360.

RACM2_230 XYOP + HO2 → OP2; THERMAL A-FACT 3.75E-13 E/R -980.

RACM2_258 XYOP + MO2 → HCHO + 2.0 HO2 + 0.368 GLY + 0.632 MGLY + 0.737 DCB1 + 0.077 DCB2 + 0.186 DCB3; THERMAL A-FACT 3.56E-14 E/R -708.

RACM2_292 XYOP + ACO3 → MO2 + HO2 + 0.368 GLY + 0.632 MGLY + 0.737 DCB1 + 0.077 DCB2 + 0.186 DCB3; THERMAL A-FACT 7.40E-13 E/R -765.

RACM2_318 XYOP + NO3 → HO2 + 0.368 GLY + 0.632 MGLY + 0.737 DCB1 + 0.077 DCB2 + 0.186 DCB3 + NO2; THERMAL A-FACT 1.20E-12 E/R 0.0

RACM2_107 XYLP + NO → 0.95 DCB2 + 0.95 NO2 + 0.95 HO2 + 0.050 ONIT; THERMAL A-FACT 2.70E-12 E/R -360.

RACM2_260 XYLP + MO2 → HCHO + 2.0 HO2 + DCB2; THERMAL A-FACT 3.56E-14 E/R -708.

RACM2_294 XYLP + ACO3 → DCB2 + MO2 + HO2; THERMAL A-FACT 7.40E-13 E/R -765.

RACM2_333 XYLP + NO3 → DCB2 + NO2 + HO2; THERMAL A-FACT 1.20E-12 E/R 0.0

RACM2_108 PER2 + NO → 0.95 DCB1 + 0.95 NO2 + 0.95 MGLY + 0.95 HO2 + 0.050 ONIT + 1.95 DCB3; THERMAL A-FACT 2.70E-12 E/R -360.

RACM2_261 PER2 + MO2 → HCHO + 2.0 HO2 + MGLY + DCB1 + 2.05 DCB3; THERMAL A-FACT 3.56E-14 E/R -708.
RACM2_289 PER2 + ACO3 → DCB1 + MO2 + MGLY + HO2 + 2.05 DCB3; THERMAL A-FACT 7.40E-13 E/R -765.
RACM2_334 PER2 + NO3 → DCB1 + NO2 + MGLY + HO2 + 2.05 DCB3; THERMAL A-FACT 1.20E-12 E/R 0.0

Terpene Reactions

SAPRC07<BL16> TERP + OH → 0.759*xHO2 + 0.042*xRCO3 + 1.147*RO2C + 0.2*RO2XC + 0.2*zRNO3 + 0.001*xCO + 0.264*xHCHO + 0.533*xRCHO + 0.036*xACET + 0.005*xMEK + 0.009*xMGLY + 0.014*xBACL + 0.002*xMVK + 0.001*xIPRD + 0.255*xPROD2 + yR6OOH + 5.056*XC # 1.87e-11 @ -435

CB_05_R150 TERP + OH → 0.750*HO2 + 1.250*XO2 + 0.250*XO2N + 0.280*FORM + 1.66*PAR + 0.470*ALDX 1.5E-11 @ -449 20

RACM2_085 API + HO → APIP; THERMAL A-FACT 1.21E-11 E/R -440.0

RACM2_204 APIP + NO → 0.82 HO2 + 0.43 ALD + 0.82 NO2 + 0.44 KET + 0.18 ONIT + 0.23 HCHO + 0.11 ACT + 0.07 ORA1; THERMAL A-FACT 4.00E-12 E/R 0.0

RACM2_227 APIP + HO2 → OP2; THERMAL A-FACT 1.50E-11 E/R 0.0

RACM2_252 APIP + MO2 → HO2 + 0.750 ALD + 0.750 HCHO + 0.750 KET + 0.250 MOH + 0.250 ROH; THERMAL A-FACT 3.56E-14 E/R -708.0

RACM2_283 APIP + ACO3 → 0.5 HO2 + ALD + 0.5 MO2 + KET + ORA2; THERMAL A-FACT 7.40E-13 E/R -765.0

RACM2_315 APIP + NO3 → HO2 + ALD + NO2 + KET; THERMAL A-FACT 1.20E-12 E/R 0.0

RACM2_086 LIM + HO → LIMP; THERMAL A-FACT 4.20E-11 E/R -401.0

RACM2_205 LIMP + NO → 0.90 HO2 + 0.25 MACR + 0.25 KET + 0.03 ACT + 0.90 NO2 + 0.10 ONIT; THERMAL A-FACT 4.00E-12 E/R 0.0

RACM2_228 LIMP + HO2 → OP2; THERMAL A-FACT 1.50E-11 E/R 0.0

RACM2_253 LIMP + MO2 → HO2 + 0.308 MACR + 0.192 OLI + 1.04 HCHO + 0.250 MOH + 0.250 ROH; THERMAL A-FACT 3.56E-14 E/R -708.0

RACM2_284 LIMP + ACO3 → 0.5 HO2 + 0.308 MACR + 0.192 OLI + 0.385 HCHO + 0.5 MO2 + 0.5 ORA2; THERMAL A-FACT 7.40E-13 E/R -765.0

RACM2_316 LIMP + NO3 → HO2 + 0.615 MACR + 0.385 OLI + 0.385 HCHO + NO2; THERMAL A-FACT 1.20E-12 E/R 0.0

SAPRC07<BL17> TERP + O3 → 0.052*HO2 + 0.067*xHO2 + 0.585*OH + 0.126*xMECO3 + 0.149*xRCO3 + 0.875*RO2C + 0.203*RO2XC + 0.203*zRNO3 + 0.166*CO + 0.019*xCO + 0.045*CO2 + 0.079*HCHO + 0.15*xHCHO + 0.22*xRCHO + 0.165*xACET + 0.004*MEK + 0.107*FACD + 0.043*PACD + 0.001*xGLY + 0.002*xMGLY + 0.055*xBACL + 0.001*xMACR + 0.001*xIPRD + 0.409*PRD2 + 0.545*yR6OOH + 3.526*XC # 9.57e-16 @ 785

CB_05_R151 TERP + O3 → 0.570*OH + 0.070*HO2 + 0.760*XO2 + 0.180*XO2N + 0.240*FORM + 0.001*CO + 7.000*PAR + 0.210*ALDX + 0.390*CXO3 1.2E-15 @ 821

RACM2_180 API + O3 → 0.65 ALD + 0.53 KET + 0.14 CO + 0.20 ETHP + 0.42 KETP + 0.85 HO + 0.10 HO2 + 0.02 H2O2; THERMAL A-FACT 5.00E-16 E/R 530.0
RACM2_181 LIM + O3 → 0.04 HCHO + 0.46 OLت + 0.14 CO + 0.16 ETHP + 0.42 KETP + 0.85 HO + 0.10 HO2 + 0.02 H2O2 + 0.79 MACR + 0.01 ORA1 + 0.07 ORA2; THERMAL A-FACT 2.95E-15 E/R 783.0

SAPRC07<BL18> TERP + NO3 → 0.162*xHO2 + 0.421*xNO2 + 0.019*xRCO3 + 1.509*RO2C + 0.397*RO2XC + 0.397*zRNO3 + 0.01*xCO + 0.017*xHCHO + 0.001*xCCHO + 0.509*xRCHO + 0.175*xACET + 0.001*xMGLY + 0.003*xMACR + 0.001*xMVK + 0.002*xIPRD + 0.163*xRNO3 + yR6OOH + 0.416*XN + 4.473*XC # 1.28e-12@-490
CB_05_R152 TERP + NO3 → 0.470*NO2 + 0.280*HO2 + 1.030*XO2 + 0.250*XO2N + 0.470*ALDX + 0.530*NTR 3.7E-12 @ -175

RACM2_169 API + NO3 → 0.10 OLNN + 0.90 OLND; THERMAL A-FACT 1.19E-12 E/R -490.0
RACM2_170 LIM + NO3 → 0.13 OLNN + 0.87 OLND; THERMAL A-FACT 1.22E-11 E/R 0.0

SAPRC07<BL19> TERP + O3P → 0.147*RCHO + 0.853*PRD2 + 4.441*XC # 3.71e-11
CB_05_R149 TERP + O → 0.150*ALDX + 5.12*PAR 3.60E-11 20
RACM2_000 No Equivalent

SAPRC Chlorine Reactions

SAPRC07<CI01> CL2 → 2*CL # 1.0/SAPRC07<CL2>
CB_05_000 No Equivalent
RACM2_000 No Equivalent

SAPRC07<CI02> CL + NO + M → CLNO # 7.60e-32^-1.80
CB_05_000 No Equivalent
RACM2_000 No Equivalent

SAPRC07<CI03> CLNO → CL + NO # 1.0/SAPRC07<CLNO-06>
CB_05_000 No Equivalent
RACM2_000 No Equivalent

SAPRC07<CI04> CL + NO2 → CLONO # 1.30e-30^-2.00&1.00e-10^-1.00&0.60&1.0
CB_05_000 No Equivalent
RACM2_000 No Equivalent

SAPRC07<CI05> CL + NO2 → CLNO2 # 1.80e-31^-2.00&1.00e-10^-1.00&0.60&1.0

CB_05_000 No Equivalent
RACM2_000 No Equivalent

SAPRC07<CI06> CLONO → CL + NO2 # 1.0/SAPRC07<CLONO>
CB_05_000 No Equivalent
RACM2_000 No Equivalent

SAPRC07<CI07> CLNO2 → CL + NO2 # 1.0/SAPRC07<CLNO2>
CB_05_000 No Equivalent
RACM2_000 No Equivalent

SAPRC07<CI08> CL + HO2 → HCL # 3.44e-11^-0.56
CB_05_000 No Equivalent
RACM2_000 No Equivalent

SAPRC07<CI09> CL + HO2 → CLO + OH # 9.41e-12^2.10
CB_05_000 No Equivalent
RACM2_000 No Equivalent

SAPRC07<CI10> CL + O3 → CLO # 2.80e-11@250
CB_05_000 No Equivalent
RACM2_000 No Equivalent

SAPRC07<CI11> CL + NO3 → CLO + NO2 # 2.40e-11
CB_05_000 No Equivalent
RACM2_000 No Equivalent

SAPRC07<CI12> CLO + NO → CL + NO2 # 6.20e-12@-295
CB_05_000 No Equivalent
RACM2_000 No Equivalent

SAPRC07<CI13> CLO + NO2 → CLONO2 # 1.80e-31^-3.40&1.50e-11^-1.90&0.60&1.0
CB_05_000 No Equivalent
RACM2_000 No Equivalent

SAPRC07<CI14> CLONO2 → CLO + NO2 # 1.0/SAPRC07<CLONO2-1>

CB_05_000 No Equivalent
RACM2_000 No Equivalent

SAPRC07<CI15> CLONO2 → CL + NO3 # 1.0/SAPRC07<CLONO2-2>
CB_05_000 No Equivalent
RACM2_000 No Equivalent

SAPRC07<CI16> CLONO2 → CLO + NO2 # 4.48e-05^-1.00@12530&3.71e+15^3.50@12530&0.60&1.0
CB_05_000 No Equivalent
RACM2_000 No Equivalent

SAPRC07<CI17> CL + CLONO2 → CL2 + NO3 # 6.20e-12@-145
CB_05_000 No Equivalent
RACM2_000 No Equivalent

SAPRC07<CI18> CLO + HO2 → HOCL # 2.20e-12@-340
CB_05_000 No Equivalent
RACM2_000 No Equivalent

SAPRC07<CI19> HOCL → OH + CL # 1.0/SAPRC07<HOCL-06>
CB_05_000 No Equivalent
RACM2_000 No Equivalent

SAPRC07<CI20> CLO + CLO → 0.29*CL2 + 1.42*CL # 1.25e-11@1960
CB_05_000 No Equivalent
RACM2_000 No Equivalent

SAPRC07<CI21> OH + HCL → CL # 1.70e-12@230
CB_05_000 No Equivalent
RACM2_000 No Equivalent

SAPRC07<CI22> CL + H2 → HCL + HO2 # 3.90e-11@2310
CB_05_000 No Equivalent
RACM2_000 No Equivalent

SAPRC07<CP01> HCHO + CL → HCL + HO2 + CO # 8.10e-11@30

CB_05_000 No Equivalent

RACM2_000 No Equivalent

SAPRC07<CP02> CCHO + CL → HCL + MECO3 # 8.00e-11

CB_05_000 No Equivalent

RACM2_000 No Equivalent

SAPRC07<CP03> MEOH + CL → HCL + HCHO + HO2 # 5.50e-11

CB_05_000 No Equivalent

RACM2_000 No Equivalent

SAPRC07<CP04> RCHO + CL → HCL + 0.9*RCO3 + 0.1*RO2C + 0.1*xCCHO + 0.1*xCO + 0.1*xHO2 + 0.1*yROOH # 1.23e-10

CB_05_000 No Equivalent

RACM2_000 No Equivalent

SAPRC07<CP05> ACET + CL → HCL + RO2C + xHCHO + xMECO3 + yROOH # 7.70e-11@1000

CB_05_000 No Equivalent

RACM2_000 No Equivalent

SAPRC07<CP06> MEK + CL → HCL + 0.975*RO2C + 0.039*RO2XC + 0.039*zRNO3 + 0.84*xHO2 + 0.085*xMECO3 + 0.036*xRCO3 + 0.065*xHCHO + 0.07*xCCHO + 0.84*xRCHO + yROOH + 0.763*XC # 3.60e-11

CB_05_000 No Equivalent

RACM2_000 No Equivalent

SAPRC07<CP07> RNO3 + CL → HCL + 0.038*NO2 + 0.055*HO2 + 1.282*RO2C + 0.202*RO2XC + 0.202*zRNO3 + 0.009*RCHO + 0.018*MEK + 0.012*PRD2 + 0.055*RNO3 + 0.159*xNO2 + 0.547*xHO2 + 0.045*xHCHO + 0.3*xCCHO + 0.02*xRCHO + 0.003*xACET + 0.041*xMEK + 0.046*xPROD2 + 0.547*xRNO3 + 0.908*yR6OOH + 0.201*XN + - 0.149*XC # 1.92e-10

CB_05_000 No Equivalent

RACM2_000 No Equivalent

SAPRC07<CP08> PRD2 + CL → HCL + 0.314*HO2 + 0.68*RO2C + 0.116*RO2XC + 0.116*zRNO3 + 0.198*RCHO + 0.116*PRD2 + 0.541*xHO2 + 0.007*xMECO3 + 0.022*xRCO3 + 0.237*xHCHO + 0.109*xCCHO + 0.591*xRCHO + 0.051*xMEK + 0.04*xPROD2 + 0.686*yR6OOH + 1.262*XC # 2.00e-10

CB_05_000 No Equivalent

RACM2_000 No Equivalent

SAPRC07<CP09> GLY + CL → HCL + 0.63*HO2 + 1.26*CO + 0.37*RCO3 + -0.37*XC # 8.10e-11@30

CB_05_000 No Equivalent

RACM2_000 No Equivalent

SAPRC07<CP10> MGLY + CL → HCL + CO + MECO3 # 8.00e-11

CB_05_000 No Equivalent

RACM2_000 No Equivalent

SAPRC07<CP11> CRES + CL → HCL + xHO2 + xBALD + yR6OOH # 6.20e-11

CB_05_000 No Equivalent

RACM2_000 No Equivalent

SAPRC07<CP12> BALD + CL → HCL + BZCO3 # 8.00e-11

CB_05_000 No Equivalent

RACM2_000 No Equivalent

SAPRC07<CP13> ROOH + CL → HCL + 0.414*OH + 0.588*RO2C + 0.414*RCHO + 0.104*xOH + 0.482*xHO2 + 0.106*xHCHO + 0.104*xCCHO + 0.197*xRCHO + 0.285*xMEK + 0.586*yROOH + -0.287*XC # 1.66e-10

CB_05_000 No Equivalent

RACM2_000 No Equivalent

SAPRC07<CP14> R6OOH + CL → HCL + 0.145*OH + 1.078*RO2C + 0.117*RO2XC + 0.117*zRNO3 + 0.145*PRD2 + 0.502*xOH + 0.237*xHO2 + 0.186*xCCHO + 0.676*xRCHO + 0.28*xPROD2 + 0.855*yR6OOH + 0.348*XC # 3.00e-10

CB_05_000 No Equivalent

RACM2_000 No Equivalent

SAPRC07<CP15> RAOOH + CL → 0.404*HCL + 0.045*OH + 0.192*HO2 + 0.63*RO2C + 0.132*RO2XC + 0.132*zRNO3 + 0.1*PRD2 + 0.093*MGLY + 0.045*IPRD + 0.032*xOH + 0.598*xHO2 + 0.594*xRCHO + 0.021*xMEK + 0.205*xMGLY + 0.021*xAFG1 + 0.021*xAFG2 + 0.763*yR6OOH + 3.413*XC # 4.29e-10

CB_05_000 No Equivalent

RACM2_000 No Equivalent

SAPRC07<CP16> MACR + CL → 0.25*HCL + 0.165*MACO3 + 0.802*RO2C + 0.033*RO2XC + 0.033*zRNO3 + 0.802*xHO2 + 0.541*xCO + 0.082*xIPRD + 0.18*xCLCCHO + 0.541*xCLACET + 0.835*yROOH + 0.208*XC # 3.85e-10

CB_05_000 No Equivalent

RACM2_000 No Equivalent

SAPRC07<CP17> MVK + CL → 1.283*RO2C + 0.053*RO2XC + 0.053*zRNO3 + 0.322*xHO2 + 0.625*xMECO3 + 0.947*xCLCCHO + yROOH + 0.538*XC # 2.32e-10

CB_05_000 No Equivalent

RACM2_000 No Equivalent

SAPRC07<CP18> IPRD + CL → 0.401*HCL + 0.084*HO2 + 0.154*MACO3 + 0.73*RO2C + 0.051*RO2XC + 0.051*zRNO3 + 0.042*AFG1 + 0.042*AFG2 + 0.712*xHO2 + 0.498*xCO + 0.195*xHCHO + 0.017*xMGLY + 0.009*xAFG1 + 0.009*xAFG2 + 0.115*xIPRD + 0.14*xCLCCHO + 0.42*xCLACET + 0.762*yR6OOH + 0.709*XC # 4.12e-10

CB_05_000 No Equivalent

RACM2_000 No Equivalent

SAPRC07<CP19> CLCCHO → HO2 + CO + RO2C + xCL + xHCHO + yROOH # 1.0/SAPRC07<CLCCHO>

CB_05_000 No Equivalent

RACM2_000 No Equivalent

SAPRC07<CP20> CLCCHO + OH → RCO3 + -1*XC # 3.10e-12

CB_05_000 No Equivalent

RACM2_000 No Equivalent

SAPRC07<CP21> CLCCHO + CL → HCL + RCO3 + -1*XC # 1.29e-11

CB_05_000 No Equivalent

RACM2_000 No Equivalent

SAPRC07<CP22> CLACET → MECO3 + RO2C + xCL + xHCHO + yROOH # 5.00e-1/SAPRC07<CLACET>

CB_05_000 No Equivalent

RACM2_000 No Equivalent

SAPRC07<CP23> xCL → CL # 'RO2RO'

CB_05_000 No Equivalent

RACM2_000 No Equivalent

SAPRC07<CP24> xCL → # 'RO2XRO'

CB_05_000 No Equivalent

RACM2_000 No Equivalent

SAPRC07<CP25> xCLCCHO → CLCCHO # 'RO2RO'

CB_05_000 No Equivalent

RACM2_000 No Equivalent

SAPRC07<CP26> xCLCCHO → 2*XC # 'RO2XRO'

CB_05_000 No Equivalent

RACM2_000 No Equivalent

SAPRC07<CP27> xCLACET → CLACET # 'RO2RO'

CB_05_000 No Equivalent

RACM2_000 No Equivalent

SAPRC07<CP28> xCLACET → 3*XC # 'RO2XRO'

CB_05_000 No Equivalent

RACM2_000 No Equivalent

SAPRC07<CE01> CH4 + CL → HCL + MEO2 # 7.30e-12@1280

CB_05_000 No Equivalent

RACM2_000 No Equivalent

SAPRC07<CE02> ETHE + CL → 2*RO2C + xHO2 + xHCHO + CLCHO # 1.60e-29^3.30&3.10e-10^-1.00&0.60&1.0

CB_05_000 No Equivalent

RACM2_000 No Equivalent

SAPRC07<CE03> ISOP + CL → 0.15*HCL + 1.168*RO2C + 0.085*RO2XC + 0.085*zRNO3 + 0.738*xHO2 + 0.177*xCL + 0.275*xHCHO + 0.177*xMVK + 0.671*xIPRD + 0.067*xCLCCHO + yR6OOH + 0.018*XC # 4.80e-10

CB_05_000 No Equivalent

RACM2_000 No Equivalent

SAPRC07<CE04> ACYE + CL → HO2 + CO + XC # 5.20e-30^-2.40&2.20e-10&0.60&1.0

CB_05_000 No Equivalent

RACM2_000 No Equivalent

SAPRC07<CL01> ALK1 + CL → xHO2 + RO2C + HCL + xCCHO + yROOH # 8.30e-11@100

CB_05_000 No Equivalent

RACM2_000 No Equivalent

SAPRC07<CL02> ALK2 + CL → 0.97*xHO2 + 0.97*RO2C + 0.03*RO2XC + 0.03*zRNO3 + HCL + 0.482*xRCHO + 0.488*xACET + yROOH + -0.09*XC # 1.20e-10@-40

CB_05_000 No Equivalent

RACM2_000 No Equivalent

SAPRC07<CL03> ALK3 + CL → 0.835*xHO2 + 0.094*xTBUO + 1.361*RO2C + 0.07*RO2XC + 0.07*zRNO3 + HCL + 0.078*xHCHO + 0.34*xCCHO + 0.343*xRCHO + 0.075*xACET + 0.253*xMEK + 0.983*yROOH + 0.017*yR6OOH + 0.18*XC # 1.86e-10

CB_05_000 No Equivalent

RACM2_000 No Equivalent

SAPRC07<CL04> ALK4 + CL → 0.827*xHO2 + 0.003*xMEO2 + 0.004*xMEO3 + 1.737*RO2C + 0.165*RO2XC + 0.165*zRNO3 + HCL + 0.003*xCO + 0.034*xHCHO + 0.287*xCCHO + 0.412*xRCHO + 0.247*xACET + 0.076*xMEK + 0.13*xPROD2 + yR6OOH + 0.327*XC # 2.63e-10

CB_05_000 No Equivalent

RACM2_000 No Equivalent

SAPRC07<CL05> ALK5 + CL → 0.647*xHO2 + 1.541*RO2C + 0.352*RO2XC + 0.352*zRNO3 + HCL + 0.022*xHCHO + 0.08*xCCHO + 0.258*xRCHO + 0.044*xACET + 0.041*xMEK + 0.378*xPROD2 + yR6OOH + 2.368*XC # 4.21e-10

CB_05_000 No Equivalent

RACM2_000 No Equivalent

SAPRC07<CL06> OLE1 + CL → 0.902*xHO2 + 1.42*RO2C + 0.098*RO2XC + 0.098*zRNO3 + 0.308*HCL + 0.025*xHCHO + 0.146*xCCHO + 0.051*xRCHO + 0.188*xMACR + 0.014*xMVK + 0.027*xIPRD + 0.225*xCLCCHO + 0.396*xCLACET + 0.413*yROOH + 0.587*yR6OOH + 1.361*XC # 3.55e-10

CB_05_000 No Equivalent

RACM2_000 No Equivalent

SAPRC07<CL07> OLE2 + CL → 0.447*xHO2 + 0.448*xCL + 0.001*xMEO2 + 1.514*RO2C + 0.104*RO2XC + 0.104*zRNO3 + 0.263*HCL + 0.228*xHCHO + 0.361*xCCHO + 0.3*xRCHO + 0.081*xACET + 0.04*xMEK +

**0.049*xMACR + 0.055*xMVK + 0.179*xIPRD + 0.012*xCLCCHO + 0.18*xCLACET + 0.357*yROOH + 0.643*yR6OOH +
0.247*XC # 3.83e-10**

CB_05_000 No Equivalent

RACM2_000 No Equivalent

**SAPRC07<CL08> ARO1 + CL → 0.88*xHO2 + 0.88*RO2C + 0.12*RO2XC + 0.12*zRNO3 + 0.671*xBALD +
0.21*xPROD2 + 0.323*XC # 1.00e-10**

CB_05_000 No Equivalent

RACM2_000 No Equivalent

**SAPRC07<CL09> ARO2 + CL → 0.842*xHO2 + 0.842*RO2C + 0.158*RO2XC + 0.158*zRNO3 + 0.618*xBALD +
0.224*xPROD2 + 2.382*XC # 2.18e-10**

CB_05_000 No Equivalent

RACM2_000 No Equivalent

**SAPRC07<CL10> TERP + CL → 0.252*xHO2 + 0.068*xCL + 0.034*xMECO3 + 0.05*xRCO3 + 0.016*xMACO3 +
2.258*RO2C + 0.582*RO2XC + 0.582*zRNO3 + 0.548*HCL + 0.035*xCO + 0.158*xHCHO + 0.185*xRCHO +
0.274*xACET + 0.007*xGLY + 0.003*xBACL + 0.003*xMVK + 0.158*xIPRD + 0.006*xAFG1 + 0.006*xAFG2 +
0.001*xAFG3 + 0.109*xCLCCHO + yR6OOH + 3.543*XC # 5.46e-10**

CB_05_000 No Equivalent

RACM2_000 No Equivalent

Reactions Unique to CB05

O3P Atom Reactions

CB_05_R40 OH + O → HO2 2.2E-11 @ -120
CB_05_R44 HO2 + O → OH 3.0E-11 @ -200
CB_05_R45 H2O2 + O → OH + HO2 1.4E-12 @ 2000
CB_05_R46 NO3 + O → NO2 1.00E-11
CB_05_R76 FORM + O → OH + HO2 + CO 3.4E-11 @ 1600
CB_05_R83 ALD2 + O → C2O3 + OH 1.8E-11 @ 1100
CB_05_R98 ALDX+O → CXO3 + OH 1.3E-11 @ 870

O1D Atom Reactions

CB_05_R38 O1D + H2 → OH + HO2 1.10E-10

Nitrogen Compound Reactions

Photolysis

CB_05_R53 N2O5 + hv → NO2 + NO3 1.0 x <N2O5_IUPAC05>
CB_05_R62 NTR + hv → NO2 + HO2 + 0.330*FORM + 0.330*ALD2 + 0.330*ALDX – 0.660*PAR 1.0 x <NTR_IUPAC05>

Thermal Reactions

CB_05_R23 NO + NO2 + H2O → 2*HONO 5.00E-40
CB_05_R27 HONO + HONO → NO + NO2 1.00E-20
CB_05_R49 NO3 + O3 → NO2 1.00E-17

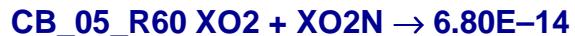
Radical-Radical Reactions

CB_05_R41 OH + OH → O 4.2E-12 @ 240
CB_05_R42 OH + OH → H2O2 6.9E-31^-1.0 & 2.6E-11^0
CB_05_R81 HCO3 + HO2 → MEPX 5.6E-15 @ -2300

Secondary Alkoxy Radical Reactions

CB_05_R113 ROR → 0.960*XO2 + 0.600*ALD2 + 0.940*HO2 – 2.100*PAR + 0.040*XO2N + 0.020*ROR + 0.500*ALDX 1.0E+15 @ 8000
CB_05_R114 ROR → HO2 1.60E+03
CB_05_R115 ROR + NO2 → NTR 1.50E-11

Peroxy Operator Reactions



PANs



Ethanol



Isoprene Products

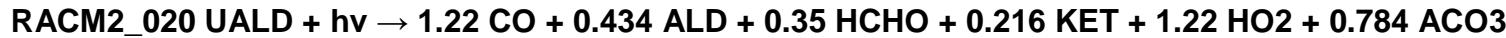


CB05 and RACM2



Reactions Unique to RACM2

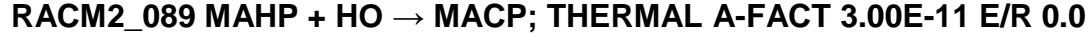
Photolysis



Propanol



Reactions of Products with HO



RACM2_092 ETEG + HO → ALD + HO₂; THERMAL A-FACT 1.47E-11 E/R 0.0

RACM2_143 PAN + HO → HCHO + NO₃ + XO₂ + H₂O; THERMAL A-FACT 4.00E-14 E/R 0.

RACM2_144 PPN + HO → HCHO + NO₃ + XO₂ + H₂O; THERMAL A-FACT 4.00E-14 E/R 0.

RACM2_145 MPAN + HO → HACE + NO₂; THERMAL A-FACT 3.20E-11 E/R 0.

RACM2 Peroxy Radical Reactions

RACM2_122 MCTP + HO₂ → OP₂; THERMAL A-FACT 3.75E-13 E/R -980.

RACM2_120 MCTP + MO₂ → HCHO + HO₂ + MCTO; THERMAL A-FACT 3.56E-14 E/R -708.

RACM2_121 MCTP + ACO₃ → MO₂ + HO₂ + MCTO; THERMAL A-FACT 7.40E-13 E/R -708.

RACM2 Nitrate Radical Reactions

RACM2_154 EPX + NO₃ → 1.50 HO₂ + 0.50 HO + 1.50 CO + GLY + 0.50 CO₂ + 0.50 NO₂ + 0.50 HNO₃;

THERMAL A-FACT 2.87E-13 E/R 1000.0

RACM2_168 UALD + NO₃ → 0.668 CO + 0.332 HCHO + 0.332 ALD + ONIT + HO₂ + X0₂; THERMAL A-FACT 5.02E-13 E/R 1076.0

RACM2_171 MPAN + NO₃ → MACP + NO₂; THERMAL A-FACT 2.20E-14 E/R 500.0